



# Introduction to stochastic calculus and to the resolution of PDEs using Monte Carlo simulations - Lectures notes of XV Spanish-French School on Numerical Simulation in Physics and Engineering

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# Introduction to stochastic calculus and to the resolution of PDEs using Monte Carlo simulations

These lecture notes are provided for the personal use of participants of the *XV Spanish-French School on Numerical Simulation in Physics and Engineering*, to be held in Torremolinos, Málaga (Spain) on September 24-28, 2012.

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## Abstract

I give a pedagogical introduction to Brownian motion, stochastic calculus introduced by Ito in the fifties, following the elementary (at least not too technical) approach by Föllmer [Föl81]. Based on this, I develop the connection with linear and semi-linear parabolic PDEs. Then, I provide and analyze some Monte Carlo methods to approximate the solution to these PDEs

This course is aimed at master students, PhD students and researchers interesting in the connection of stochastic processes with PDEs and their numerical counterpart. The reader is supposed to be familiar with basic concepts of probability (say first chapters of the book *Probability essentials* by Jacod and Protter [JP03]), but no a priori knowledge on martingales and stochastic processes is required.

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# 1 The Brownian motion and related processes

## 1.1 A brief history of Brownian motion

Historically, the Brownian motion (BM in short) is associated with the analysis of motions which time evolution is so disordered that it seems difficult to forecast their evolution, even in a very short time interval. It plays a central role in the theory of random processes, because in many theoretical and applied problems, the Brownian motion (or the diffusion processes that are built from BM) provides simple limit models on which many calculations can be made.

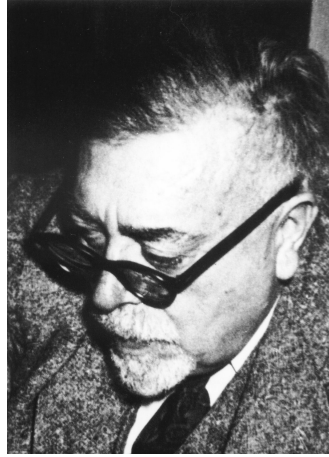


Robert Brown (1773-1858)

In 1827, the English botanist Robert Brown (1773-1858) first described the erratic motion of fine organic particles in suspension in a gas or a fluid. At the XIX<sup>th</sup> century, after him, several physicists had admitted that this motion is very irregular and does not seem to admit a tangent; thus one could not speak of his speed, nor apply the laws of mechanics to him! In 1900 [Bac00], Louis Bachelier (1870-1946) introduced the Brownian motion to model the dynamics of the stock prices, but his approach then is forgotten until the sixties... His PhD thesis, *Théorie de la spéculation*, is the starting point of modern finance.

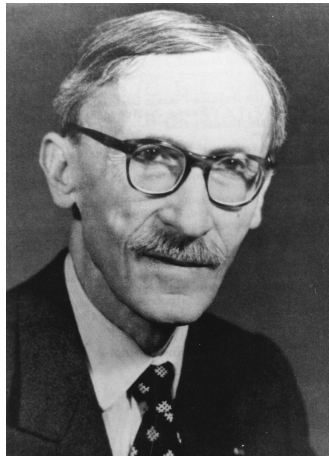
But Physics is the field at the beginning of the XX<sup>th</sup> century which is at the origin of great interest for this process. In 1905, Albert Einstein (1879-1955) built a probabilistic model to describe the motion of a diffusive particle: he found that the law of the particle position at the time  $t$ , given the initial state  $x$ , admits a density which satisfies to the *heat equation*, and actually it is *Gaussian*. Its theory is then quickly confirmed by experimental measurements of satisfactory diffusion constants. The same year as Einstein, a discrete

version of the Brownian motion is proposed by the Polish physicist Smoluchowski using random walks.



Norbert Wiener<sup>1</sup> (1894-1964).

In 1923, Norbert Wiener (1894-1964) built rigorously the random function that is called *Brownian motion*; he established in particular that the trajectories are continuous. By 1930, while following an idea of Paul Langevin, Ornstein and Uhlenbeck studied the Gaussian random function which bears their name and which seems to be the stationary or mean-reverting equivalent model associated to the Brownian motion.



Paul Lévy (1886-1971)

It is the beginning of a very active theoretical research in Mathematics. Paul Lévy (1886-1971) discovered then, with other mathematicians, many properties of the Brownian motion [Lév39] and introduced a first form of the stochastic differential equations, which study is later systematized by K. Itô (1915-2008). His work is gathered in a famous treaty published in 1948 [Ito51] which is usually referred to as *Itô stochastic calculus*.

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<sup>1</sup>The pictures of Wiener-Lévy-Itô are from archives of "Mathematisches Forschungsinstitut Oberwolfach".



Kiyosi Itô (1915-2008)

But History knows sometimes incredible bounces. Indeed in 2000, the French Academy of Science opened a manuscript remained sealed since 1940 pertaining to the young mathematician Doebelin (1915-2008), a French telegraphist died during the German offensive. Doebelin was already known for his remarkable achievements in the theory of probability due to his works on the stable laws and the Markov processes. This sealed manuscript gathered in fact his recent research, written between November 1939 and February 1940: it was actually related to his discovery (before Itô) of the stochastic differential equations and their relations with the Kolmogorov partial differential equations. Perhaps the Itô stochastic calculus could have been called Doebelin stochastic calculus...

## 1.2 The Brownian motion and its paths

In the following, we study the basic properties of the Brownian motion and its paths.

### 1.2.1 Definition and existence

The very erratic path which is a specific feature of the Brownian motion is in general associated with the observation that the phenomenon, although very disordered, has a certain time homogeneity, i.e. the origin date does not have importance to describe the time evolution. These properties underly the next definition.

**Definition 1.1 (of standard Brownian motion)** *A standard Brownian motion is a random process  $\{W_t; t \geq 0\}$  with continuous paths, such that*

- $W_0 = 0$ ;
- *the time increment  $W_t - W_s$  with  $0 \leq s < t$  has the Gaussian law<sup>2</sup>, with zero mean and variance equal  $(t - s)$ ;*

---

<sup>2</sup>A Gaussian random variable  $X$  with mean  $\mu$  and variance  $\sigma^2 > 0$  (often denoted by  $\mathcal{N}(\mu, \sigma^2)$ ) is the r.v. with density

$$g_{\mu, \sigma^2}(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left[-\frac{(x - \mu)^2}{2\sigma^2}\right], \quad x \in \mathbb{R}.$$

If  $\sigma^2 = 0$ ,  $X = \mu$  with probability 1. Moreover, for any  $u \in \mathbb{R}$ ,  $\mathbb{E}(e^{uX}) = e^{u\mu + \frac{1}{2}u^2\sigma^2}$ .

- for any  $0 = t_0 < t_1 < t_2 \dots < t_n$ , the increments  $\{W_{t_{i+1}} - W_{t_i}; 0 \leq i \leq n-1\}$  are independent<sup>3</sup> random variables.

There are important remarks following from the definition.

1. The state  $W_t$  of the system at time  $t$  is distributed as a Gaussian r.v. with mean 0 and variance  $t$  (increasing as time gets larger). Its probability density is

$$\mathbb{P}(W_t \in [x, x + dx]) = g(t, x)dx = \frac{1}{\sqrt{2\pi t}} \exp(-x^2/2t)dx. \quad (1.1)$$

2. With probability 95%, we have  $|W_t| \leq 1.96\sqrt{t}$  (see Figure 1.1) for a given time  $t$ . However, it may occur that  $W$  goes out this confidence interval.



Figure 1.1: Simulation of a BM with the 95%-confidence interval curves  $f_{\pm}(t) = \pm 2\sqrt{t}$ .

3. The random variable  $W_t$ , as the sum of its increments, can be decomposed as a sum of independent Gaussian r.v.: this property serves as a basis from the further stochastic calculus.

### Theorem 1.2 *The Brownian motion exists!*

PROOF :

There are different constructive ways to prove the existence of BM. Here, we use a Fourier based approach, showing that  $W$  can be represented as a superposition of Gaussian signals. Also, we use an equivalent characterization of BM as a Gaussian process<sup>4</sup> with zero mean and covariance function  $\text{Cov}(W_t, W_s) = \min(s, t) = s \wedge t$ .

<sup>3</sup>Two random variables  $X_1$  and  $X_2$  are independent if and only if  $\mathbb{E}(f(X_1)g(X_2)) = \mathbb{E}(f(X_1))\mathbb{E}(g(X_2))$  for any bounded functions  $f$  and  $g$ . This extends similarly to a vector.

<sup>4</sup> $(X_1, \dots, X_n)$  is a Gaussian vector if and only if for any  $(\lambda_i)_{1 \leq i \leq n} \in \mathbb{R}^n$ ,  $\sum_{i=1}^n \lambda_i X_i$  has a Gaussian distribution. Independent Gaussian random variables form a Gaussian vector. A process  $(X_t)_t$  is Gaussian if  $(X_{t_1}, \dots, X_{t_n})$  is a Gaussian vector for any times  $(t_1, \dots, t_n)$  and any  $n$ . A Gaussian process is characterized by its mean  $m(t) = \mathbb{E}(X_t)$  and its covariance function  $K(s, t) = \text{Cov}(X_s, X_t)$ .

Let  $(G_m)_{m \geq 0}$  be a sequence of independent Gaussian r.v. with zero mean and unit variance and set

$$W_t = \frac{t}{\sqrt{\pi}} G_0 + \sqrt{\frac{2}{\pi}} \sum_{m \geq 1} \frac{\sin(mt)}{m} G_m.$$

We now show that  $W$  is a BM on  $[0, \pi]$ ; then it is enough to concatenate and sum up such independent processes to get finally a BM defined on  $\mathbb{R}^+$ . We sketch the proof of our statement on  $W$ . First, the series is *a.s.*<sup>5</sup> convergent since this is a Cauchy sequence in  $L_2$ : indeed, thanks to the independence of the Gaussian random variables, we have

$$\left\| \sum_{m_1 \leq m \leq m_2} \frac{\sin(mt)}{m} G_m \right\|_{L_2}^2 = \sum_{m_1 \leq m \leq m_2} \frac{\sin^2(mt)}{m^2} \leq \sum_{m_1 \leq m} \frac{1}{m^2} \xrightarrow{m_1 \rightarrow +\infty} 0.$$

The partial sum has a Gaussian distribution, thus the *a.s.* limit<sup>6</sup> too. The same argument gives that  $W$  is a Gaussian process. It has zero mean and its covariance is the limit of the covariance of partial sums: thus

$$\text{Cov}(W_t, W_s) = \frac{ts}{\pi} + \frac{2}{\pi} \sum_{m \geq 1} \frac{\sin(mt)}{m} \frac{\sin(ms)}{m}.$$

The above series is equal to  $\min(s, t)$  for  $(s, t) \in [0, \pi]^2$ , by a standard computation of the Fourier coefficients of the function  $t \in [-\pi, \pi] \mapsto \min(s, t)$  (for  $s$  fixed).  $\square$

In many applications, it is useful to consider non standard BM.

**Definition 1.3 (of arithmetic Brownian motion)** *An arithmetic Brownian motion is a random process  $\{X_t; t \geq 0\}$  where  $X_t = x_0 + bt + \sigma W_t$  and*

- $W$  is a standard BM;
- $x_0 \in \mathbb{R}$  is the starting value of  $X$ ;
- $b \in \mathbb{R}$  is the drift parameter;
- $\sigma \in \mathbb{R}$  is the diffusion parameter.

Usually,  $\sigma$  can be taken non-negative due to the symmetry of BM (see Proposition 1.4).  $X$  is still a Gaussian process, which position  $X_t$  at time  $t$  is distributed as  $\mathcal{N}(x_0 + bt, \sigma^2 t)$ .

---

<sup>5</sup>We recall that "an event  $A$  occurs *a.s.*" (*almost surely*) if  $\mathbb{P}(\omega : \omega \in A) = 1$  or equivalently if  $\{w : w \notin A\}$  is a set of zero probability measure.

<sup>6</sup>Here, we use the following standard result: let  $(X_n)_{n \geq 1}$  be a sequence of random variables, each having the Gaussian distribution with mean  $\mu_n$  and variance  $\sigma_n^2$ . If the distribution of  $X_n$  converges, then  $(\mu_n, \sigma_n^2)$  converge to  $(\mu, \sigma^2)$ , and the limit distribution is Gaussian with mean  $\mu$  and variance  $\sigma^2$ . We recall that if  $X_n$  converges *a.s.*, then it also converges in distribution.



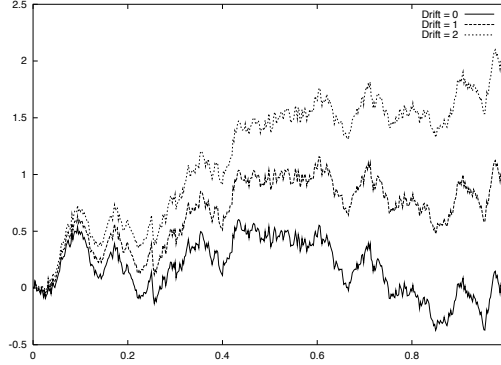


Figure 1.2: Arithmetic BM with different drift parameters.

### 1.2.2 First easy properties of the Brownian path

**Proposition 1.4** *Let  $\{W_t; t \in \mathbb{R}^+\}$  a standard BM.*

- i) SYMMETRY PROPERTY:  $\{-W_t; t \in \mathbb{R}^+\}$  is a standard BM.*
- ii) SCALING PROPERTY: for any  $c > 0$ ,  $\{W_t^c; t \in \mathbb{R}^+\}$  is a standard BM where*

$$W_t^c = c^{-1}W_{c^2t}. \quad (1.2)$$

- iii) TIME REVERSAL: for any fixed  $T$ ,  $\widehat{W}_t^T = W_T - W_{T-t}$  defines a standard BM on  $[0, T]$ .*

- iv) TIME INVERSION:  $\{\widehat{W}_t = tW_{1/t}, t > 0, \widehat{W}_0 = 0\}$  is a standard BM.*

The scaling property is important and illustrates the fractal feature of BM path:  $\varepsilon$  times  $W_t$  behaves like a BM at time  $\varepsilon^2t$ .

PROOF :

It is a direct verification of the BM definition, related to independent, stationary and Gaussian increments. The continuity is also easy to verify, except for the case *iv)* at time 0. For this, we use that  $\lim_{t \rightarrow 0^+} tW_{1/t} = \lim_{s \rightarrow +\infty} \frac{W_s}{s} = 0$ , see Proposition 1.11.  $\square$

## 1.3 Time-shift invariance and Markov property

Previously, we have studied simple spatial transformation of BM. We now consider time-shifts, by first considering deterministic shifts.

**Proposition 1.5 (Invariance by a deterministic time-shift)** *The Brownian Motion shifted by  $h \geq 0$ , given by  $\{\bar{W}_t^h = W_{t+h} - W_h; t \in \mathbb{R}^+\}$ , is another BM, independent of the Brownian Motion stopped at  $h$ ,  $\{W_s; s \leq h\}$ .*

In other words,  $\{W_{t+h} = W_h + \bar{W}_t^h; t \in \mathbb{R}^+\}$  is a BM starting from  $W_h$ . The above property is associated to the *weak Markov property* which states (possibly applicable to other processes) that *the distribution of  $W$  after  $h$  conditionally on the past up to time  $h$  depends only on the present value  $W_h$ .*

PROOF :

The Gaussian property of  $\bar{W}^h$  is clear.

The independent increments of  $W$  induce those of  $\bar{W}^h$ .

It remains to show the independence w.r.t. the past up to  $h$ , i.e. the sigma-field generated by  $\{W_s; s \leq h\}$ , or equivalently w.r.t. the sigma-field generated by  $\{W_{s_1}, \dots, W_{s_N}\}$  for any  $0 \leq s_1 \leq \dots \leq s_N \leq h$ . The independence of increments of  $W$  ensures that  $(\bar{W}_{t_1}^h, \bar{W}_{t_2}^h - \bar{W}_{t_1}^h, \dots, \bar{W}_{t_k}^h - \bar{W}_{t_{k-1}}^h) = (W_{t_1+h} - W_h, \dots, W_{t_k+h} - W_{t_{k-1}+h})$  is independent of  $(W_{s_1}, W_{s_2} - W_{s_1}, \dots, W_{s_j} - W_{s_{j-1}})$ . Then  $(\bar{W}_{t_1}^h, \bar{W}_{t_2}^h, \dots, \bar{W}_{t_k}^h)$  is independent of  $\{W_s; s \leq h\}$ .  $\square$

As a consequence, we can derive a nice symmetry result making the connection between the maximum of BM monitored along a finite time grid  $t_0 = 0 < t_1 < \dots < t_N = T$  and that of  $W_T$  only.

**Proposition 1.6** *For any  $y \geq 0$ , we have*

$$\mathbb{P}[\sup_{i \leq N} W_{t_i} \geq y] \leq 2\mathbb{P}[W_T \geq y] = \mathbb{P}[|W_T| \geq y]. \quad (1.3)$$

PROOF :

The equality at the r.h.s. comes from the symmetric distribution of  $W_T$ . Now we show the inequality on the left. Denote by  $t_y^*$  the first time  $t_j$  when  $W$  reaches the level  $y$ . Notice that  $\{\sup_{i \leq N} W_{t_i} \geq y\} = \{t_y^* \leq T\}$  and  $\{t_y^* = t_j\} = \{W_{t_i} < y, \forall i < j, W_{t_j} \geq y\}$ . For each  $j < N$ , the symmetry of Brownian increments gives  $\mathbb{P}[W_T - W_{t_j} \geq 0] = \frac{1}{2}$ . Since the shifted BM  $(\bar{W}_t^{t_j} = \bar{W}_{t_j+t} - W_{t_j} : t \in \mathbb{R}^+)$  is independent of  $(W_s : s \leq t_j)$ , we have

$$\begin{aligned} \frac{1}{2}\mathbb{P}[\sup_{i \leq N} W_{t_i} \geq y] &= \frac{1}{2}\mathbb{P}[t_y^* \leq T] = \frac{1}{2} \sum_{j=0}^N \mathbb{P}[t_y^* = t_j] \\ &= \frac{1}{2}\mathbb{P}[W_{t_i} < y, \forall i < N, W_T \geq y] + \sum_{j=0}^{N-1} \mathbb{P}[W_{t_i} < y, \forall i < j, W_{t_j} \geq y] \mathbb{P}[W_T - W_{t_j} \geq 0] \\ &= \frac{1}{2}\mathbb{P}[W_{t_i} < y, \forall i < N, W_T \geq y] + \sum_{j=0}^{N-1} \mathbb{P}[W_{t_i} < y, \forall i < j, W_{t_j} \geq y, W_T - W_{t_j} \geq 0] \\ &\leq \mathbb{P}[W_{t_i} < y, \forall i < N, W_T \geq y] + \sum_{j=0}^{N-1} \mathbb{P}[W_{t_i} < y, \forall i < j, W_{t_j} \geq y, W_T \geq y] \\ &= \mathbb{P}[t_y^* \leq T, W_T \geq y] = \mathbb{P}[W_T \geq y]. \end{aligned}$$

At the two last lines, we have used  $\{W_{t_j} \geq y, W_T - W_{t_j} \geq 0\} \subset \{W_{t_j} \geq y, W_T \geq y\}$  and  $\{W_T \geq y\} \subset \{t_y^* \leq T\}$ .  $\square$

Taking a grid with time step  $T/N$  with  $N \rightarrow +\infty$ , we have  $\sup_{i \leq N} W_{t_i} \uparrow \sup_{0 \leq t \leq T} W_t$ . Then, we can pass to the limit (up to some probabilistic convergence technicalities) in the inequality (1.3) to get

$$\mathbb{P}[\sup_{0 \leq t \leq T} W_t \geq y] \leq \mathbb{P}[|W_T| \geq y]. \quad (1.4)$$

Actually, the inequality (1.4) is an equality: it is proved later in Proposition 1.9.

Now, our aim is to extend Proposition 1.5 to the case of stochastic time-shifts  $h$ . Without extra assumption on  $h$ , the result is false in general: a counter-example is the last passage time of  $W$  at zero before the time 1 ( $L = \sup\{t \leq 1 : W_t = 0\}$ ), which does not satisfy the property. Indeed, since  $(W_{s+L} - W_s)_{s \geq 0}$  do not vanish *a.s.* at short time (due to the definition of  $L$ ), the marginal distribution can not be Gaussian and the time-shifted process can not be a BM.

The right class for extension is the class of stopping times, defined as follows.

**Definition 1.7 (Stopping time)** *A stopping time is non-negative random variable  $U$  (taking possibly the value  $+\infty$ ), such that for any  $t \geq 0$ , the event  $\{U \leq t\}$  depends only on the BM values  $\{W_s; s \leq t\}$ .*

*The stopping time is discrete if it takes only a countable set of values  $(u_1, \dots, u_n, \dots)$ .*

In other words, it suffices to observe the BM until time  $t$  to know whether or not the event  $\{U \leq t\}$  occurs. Of course, deterministic times are stopping times. A more interesting example is the first hitting time of a level  $y > 0$

$$T_y = \inf\{t > 0; W_t \geq y\};$$

it is a stopping time, since  $\{T_y \leq t\} = \{\exists s \leq t, W_s = y\}$  owing to the continuity of  $W$ . Observe that the counter-example of last passage time  $L$  is not a stopping time.

**Proposition 1.8** *Let  $U$  be a stopping time. On the event  $\{U < +\infty\}$ , the Brownian motion shifted by  $U \geq 0$ , i.e.  $\{\bar{W}_t^U = W_{t+U} - W_U; t \in \mathbb{R}^+\}$ , is a BM independent of  $\{W_t; t \leq U\}$ .*

This result is usually referred to as the *strong Markov property*.

PROOF :

We show that for any  $0 \leq t_1 < \dots < t_k$ , any  $0 \leq s_1 < \dots < s_l$ , any  $(x_1, \dots, x_k)$  and any measurable sets  $(B_1, \dots, B_{l-1})$ , we have

$$\begin{aligned} & \mathbb{P}(\bar{W}_{t_1}^U < x_1, \dots, \bar{W}_{t_k}^U < x_k, W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U < +\infty) \\ &= \mathbb{P}(W'_{t_1} < x_1, \dots, W'_{t_k} < x_k) \mathbb{P}(W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U < +\infty), \end{aligned} \quad (1.5)$$

where  $W'$  is a BM independent of  $W$ . We begin with the easier case where  $U$  is a discrete stopping time valued in  $(u_n)_{n \geq 1}$ : then

$$\begin{aligned} & \mathbb{P}(\bar{W}_{t_1}^U < x_1, \dots, \bar{W}_{t_k}^U < x_k, W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U < +\infty) \\ &= \sum_n \mathbb{P}(\bar{W}_{t_1}^{u_n} < x_1, \dots, \bar{W}_{t_k}^{u_n} < x_k, W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U, U = u_n) \\ &= \sum_n \mathbb{P}(\bar{W}_{t_1}^{u_n} < x_1, \dots, \bar{W}_{t_k}^{u_n} < x_k, W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U, U = u_n) \\ &= \sum_n \mathbb{P}(W'_{t_1} < x_1, \dots, W'_{t_k} < x_k) \mathbb{P}(W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U, U = u_n) \\ &= \mathbb{P}(W'_{t_1} < x_1, \dots, W'_{t_k} < x_k) \mathbb{P}(W_{s_1} \in B_1, \dots, W_{s_{l-1}} \in B_{l-1}, s_l \leq U < +\infty) \end{aligned}$$

applying at the last equality but one the time-shift invariance with deterministic shift  $u_n$ . For the general case for  $U$ , we apply the result to discrete stopping time  $U_n = \frac{[nU]+1}{n}$ , and then pass to the limit using the continuity of  $W$ .  $\square$

## 1.4 Maximum, behavior at infinity, path regularity

We apply the strong Markov property to identify the law of the maximum of the BM.

**Proposition 1.9 (Symmetry principle)** *For any  $y \geq 0$  and any  $x \leq y$ , we have*

$$\mathbb{P}[\sup_{t \leq T} W_t \geq y; W_T \leq x] = \mathbb{P}[W_T \geq 2y - x], \quad (1.6)$$

$$\mathbb{P}[\sup_{t \leq T} W_t \geq y] = \mathbb{P}[|W_T| \geq y] = 2 \int_{\frac{y}{\sqrt{T}}}^{+\infty} \frac{e^{-\frac{1}{2}x^2}}{\sqrt{2\pi}} dx. \quad (1.7)$$

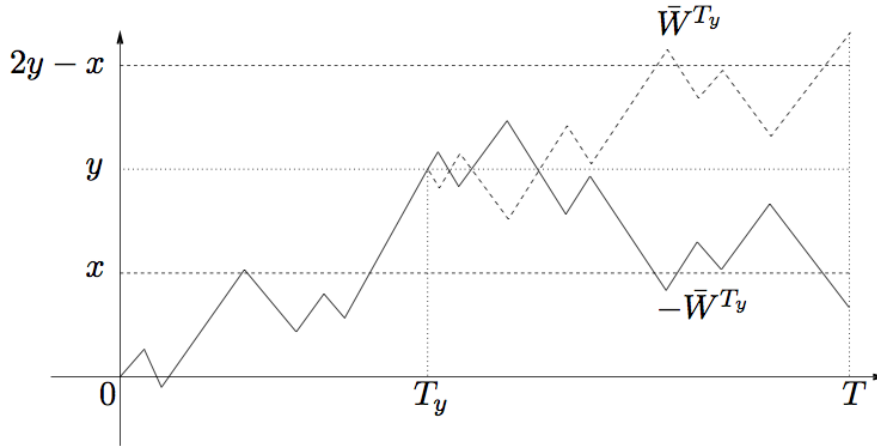


Figure 1.3: Brownian motion  $(W_{T_y+t} = \bar{W}_t^{T_y} + y : t \in \mathbb{R}^+)$  starting from  $y$  and its symmetric path.

PROOF :

Denote by  $T_y = \inf\{t > 0 : W_t \geq y\}$  and  $+\infty$  if the set is empty. Observe that  $T_y$  is a stopping time and that  $\{\sup_{t \leq T} W_t \geq y; W_T \leq x\} = \{T_y \leq T; W_T \leq x\}$ . By Proposition 1.8, on  $\{T_y \leq T\}$ ,  $(W_{T_y+t} = \bar{W}_t^{T_y} + y : t \in \mathbb{R}^+)$  is a BM starting from  $y$ , independent of  $(W_s : s \leq T_y)$ . By symmetry (see Figure 1.3), the events  $\{T_y \leq T, W_T < x\}$  and  $\{T_y \leq T, W_T > 2y - x\}$  has the same probability. But for  $x \leq y$ , we have  $\{T_y \leq T, W_T > 2y - x\} = \{W_T > 2y - x\}$  and the first result is proved.

For the second result, take  $y = x$  and write  $\mathbb{P}[\sup_{t \leq T} W_t \geq y] = \mathbb{P}[\sup_{t \leq T} W_t \geq y, W_T > y] + \mathbb{P}[\sup_{t \leq T} W_t \geq y, W_T \leq y] = \mathbb{P}[W_T > y] + \mathbb{P}[W_T \geq y] = 2\mathbb{P}(W_T \geq y) = \mathbb{P}(|W_T| \geq y)$ .  $\square$

As a consequence of the identification of the law of the maximum up to a fixed time, we prove that the range of BM becomes  $\mathbb{R}$  at time goes to infinity.

**Proposition 1.10** *With probability 1, we have*

$$\limsup_{t \rightarrow +\infty} W_t = +\infty, \quad \liminf_{t \rightarrow +\infty} W_t = -\infty.$$

PROOF :

For  $T \geq 0$ , set  $M_T = \sup_{t \leq T} W_t$ . As  $T \uparrow +\infty$ , it defines a sequence of increasing r.v., thus converging *a.s.* to a limit r.v.  $M_\infty$ . Applying twice the monotone convergence theorem, we obtain

$$\begin{aligned} \mathbb{P}[M_\infty = +\infty] &= \lim_{y \uparrow +\infty} \mathbb{P}[M_\infty > y] = \lim_{y \uparrow +\infty} \left( \lim_{T \uparrow +\infty} \mathbb{P}[M_T > y] \right) \\ &= \lim_{y \uparrow +\infty} \left( \lim_{T \uparrow +\infty} \mathbb{P}[|W_T| \geq y] \right) = 1 \end{aligned}$$

using (1.7). This proves that  $\limsup_{t \rightarrow +\infty} W_t = +\infty$  *a.s.* and a symmetry argument gives the  $\liminf$ .  $\square$

However, the increasing rate of  $W$  is sublinear as time goes to infinity.

**Proposition 1.11** *With probability 1, we have*

$$\lim_{t \rightarrow +\infty} \frac{W_t}{t} = 0.$$

PROOF :

The strong law of large numbers yields that  $\frac{W_n}{n} = \frac{1}{n} \sum_{i=1}^n (W_i - W_{i-1})$  converges *a.s.* to  $\mathbb{E}(W_1) = 0$ . The announced result is thus proved along the sequence of integers. To fill the gaps between integers, set  $\tilde{M}_n = \sup_{n < t \leq n+1} (W_t - W_n)$  and  $\tilde{M}'_n = \sup_{n < t \leq n+1} (W_n - W_t)$ : due to Proposition 1.9,  $\tilde{M}_n$  and  $\tilde{M}'_n$  have the same distribution as  $|W_1|$ . Then, the Chebyshev inequality writes

$$\mathbb{P}(|\tilde{M}_n| + |\tilde{M}'_n| \geq n^{3/4}) \leq 2 \frac{\mathbb{E}(|\tilde{M}_n|^2) + \mathbb{E}(|\tilde{M}'_n|^2)}{n^{3/2}} = 4n^{-3/2},$$

implying that  $\sum_{n \geq 0} \mathbb{P}(|\tilde{M}_n| + |\tilde{M}'_n| \geq n^{3/4}) < +\infty$ . Thus, by Borel-Cantelli's lemma, we obtain that with probability 1, for  $n$  large enough  $|\tilde{M}_n| + |\tilde{M}'_n| < n^{3/4}$ , i.e.  $\frac{\tilde{M}_n}{n}$  and  $\frac{\tilde{M}'_n}{n}$  both converge *a.s.* to 0.  $\square$

By time inversion,  $\hat{W}_t = tW_{1/t}$  is another BM: the  $\hat{W}$ -growth in infinite time gives an estimate on  $W$  at 0, which writes

$$+\infty = \limsup_{t \rightarrow +\infty} |\hat{W}_t| = \limsup_{s \rightarrow 0^+} \frac{|W_s - W_0|}{s}$$

which shows that  $W$  is not differentiable at time 0. By time-shift invariance, this is also true at any given time  $t$ . The careful reader may notice that the set of full probability measure depends on  $t$  and it is unclear at this stage if a single full set is available for any  $t$ , i.e. if

$$\mathbb{P}(\exists t_0 \text{ such that } t \mapsto W_t \text{ is differentiable at } t_0) = 0.$$

Actually, the above result holds true and it is due to Paley-Wiener-Zygmund (1933). The following result is of comparable nature: we claim that *a.s.* there does not exist any interval on which  $W$  is monotone.

**Proposition 1.12 (Nowhere monotonicity)** *We have*

$$\mathbb{P}(t \mapsto W_t \text{ is monotone on an interval}) = 0.$$

PROOF :

Define  $M_{s,t}^\uparrow = \{\omega : u \mapsto W_u(\omega) \text{ is increasing on the interval } ]s, t[ \}$  and  $M_{s,t}^\downarrow$  similarly. Observe that

$$M = \{t \mapsto W_t \text{ is monotone on the interval}\} = \bigcup_{s,t \in \mathbb{Q}, 0 \leq s < t} (M_{s,t}^\uparrow \cup M_{s,t}^\downarrow),$$

and since this is a countable union, it is enough to show  $\mathbb{P}(M_{s,t}^\uparrow) = \mathbb{P}(M_{s,t}^\downarrow) = 0$  to conclude  $\mathbb{P}(M) \leq \sum_{s,t \in \mathbb{Q}, 0 \leq s < t} [\mathbb{P}(M_{s,t}^\uparrow) + \mathbb{P}(M_{s,t}^\downarrow)] = 0$ . For fixed  $n$ , set  $t_i = s + i(t-s)/n$ , then

$$\mathbb{P}(M_{s,t}^\uparrow) \leq \mathbb{P}(W_{t_{i+1}} - W_{t_i} \geq 0, 0 \leq i < n) = \prod_{i=0}^{n-1} \mathbb{P}(W_{t_{i+1}} - W_{t_i} \geq 0) = \frac{1}{2^n},$$

leveraging the symmetric distribution of the increments. Taking now  $n$  large gives  $\mathbb{P}(M_{s,t}^\uparrow) = 0$ . We argue similarly for  $\mathbb{P}(M_{s,t}^\downarrow) = 0$ .  $\square$

In view of this lack of smoothness, it seems impossible to define differential calculus along the paths of BM. However, as it will further developed, BM paths enjoy a nice property of finite quadratic variations, which serves to build an appropriate stochastic calculus.

There are much more to tell about the properties of Brownian motion. We mention few extra properties without proof:

- **HOLDER REGULARITY:** for any  $\rho \in (0, \frac{1}{2})$  and any deterministic  $T > 0$ , there exists a *a.s.* finite r.v.  $C_{\rho,T}$  such that

$$\forall 0 \leq s, t \leq T, \quad |W_t - W_s| \leq C_{\rho,T} |t - s|^\rho.$$

- **LAW OF ITERATED LOGARITHM:** setting  $h(t) = \sqrt{2t \log \log t^{-1}}$ , we have

$$\limsup_{t \downarrow 0} \frac{W_t}{h(t)} = 1 \quad a.s. \quad \text{and} \quad \liminf_{t \downarrow 0} \frac{W_t}{h(t)} = -1 \quad a.s.$$

- **ZEROS OF BROWNIAN MOTION:** the set  $\chi = \{t \geq 0 : W_t = 0\}$  of the zeros of  $W$  is closed, unbounded, with null Lebesgue measure and it has no isolated points.

## 1.5 The random walk approximation

Another algorithmic way to build a Brownian motion consists in rescaling a random walk. This is very simple and very useful for numerics: it leads to the so-called tree methods and it has some connections with finite differences in PDEs.

Consider a sequence  $(X_i)_i$  of independent random variables with Bernoulli type distribution:  $\mathbb{P}(X_i = \pm 1) = \frac{1}{2}$ . Then

$$S_n = \sum_{i=1}^n X_i$$

defines a random walk on  $\mathbb{Z}$ . Like BM, it is a process with stationary independent increments, but it is not Gaussian. Actually  $S_n$  has a binomial distribution:

$$\mathbb{P}(S_n = -n + 2k) = \mathbb{P}(k \text{ rises}) = 2^{-n} \binom{n}{k}.$$

A direct computation shows that  $\mathbb{E}(S_n) = 0$  and  $\text{Var}(S_n) = n$ . When we rescale the walk and we let  $n$  go towards infinity, we observe however that due the Central Limit Theorem, the distribution of  $\frac{S_n}{\sqrt{n}}$  converges to the Gaussian law with zero mean and unit variance. The fact that it is equal to the law of  $W_1$  is not a coincidence, since it can be justified that the full trajectory of the suitably rescaled random walk converges towards that of a Brownian motion, see Figure 1.4. This result is known as *Donsker theorem*, see for instance [Bre92] for a proof.

**Proposition 1.13** *Define  $(Y_t^n)_t$  as the piecewise constant process*

$$Y_t^n = \frac{1}{\sqrt{n}} \sum_{i=1}^{\lfloor nt \rfloor} X_i. \quad (1.8)$$

*The distribution of the process  $(Y_t^n)_t$  converges to that of a Brownian motion  $(W_t)_t$  as  $n \rightarrow +\infty$ , i.e. for any continuous functional*

$$\lim_{n \rightarrow \infty} \mathbb{E}(\Phi(Y_t^n : t \leq 1)) = \mathbb{E}(\Phi(W_t : t \leq 1)).$$

The last result gives a simple way to evaluate numerically expectations of functionals of BM. It is the principle of the so-called *binomial tree methods*.

**Link with Finite Difference scheme.** The random walk can be interpreted as a explicit FD scheme for the heat equation. We anticipate a bit on the following where the connection between BM and heat equation will be more detailed.

For  $t = \frac{i}{n}$  ( $i \in \{0, \dots, n\}$ ) and  $x \in \mathbb{R}$ , set

$$u^n(t, x) = \mathbb{E}\left(f\left(x + Y_{\frac{i}{n}}^n\right)\right).$$

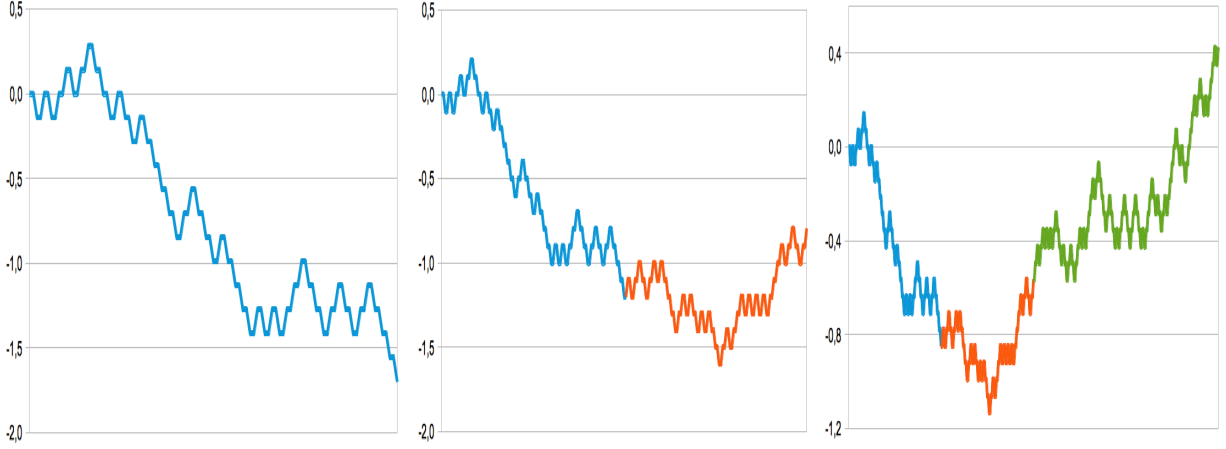


Figure 1.4: The random walk rescaled in time and space. From left to right: the process  $Y^n$  for  $n = 50, 100, 200$ . The pieces of path with same color are built with the same  $X_i$ .

The independence of  $(X_i)_i$  gives

$$\begin{aligned}
 u^n\left(\frac{i}{n}, x\right) &= \mathbb{E}\left(f\left(x + Y_{\frac{i-1}{n}}^n + \frac{X_i}{\sqrt{n}}\right)\right) \\
 &= \frac{1}{2}u^n\left(\frac{i-1}{n}, x + \frac{1}{\sqrt{n}}\right) + \frac{1}{2}u^n\left(\frac{i-1}{n}, x - \frac{1}{\sqrt{n}}\right), \\
 \frac{u^n\left(\frac{i}{n}, x\right) - u^n\left(\frac{i-1}{n}, x\right)}{\frac{1}{n}} &= \frac{1}{2} \frac{u^n\left(\frac{i-1}{n}, x + \frac{1}{\sqrt{n}}\right) - 2u^n\left(\frac{i-1}{n}, x\right) + u^n\left(\frac{i-1}{n}, x - \frac{1}{\sqrt{n}}\right)}{\left(\frac{1}{\sqrt{n}}\right)^2}.
 \end{aligned}$$

Thus,  $u^n$  related to the expectation of the random walk can be read as an explicit FD scheme of the heat equation  $\partial_t u(t, x) = \frac{1}{2} \partial_{xx}^2 u(t, x)$  and  $u(0, x) = f(x)$ , with time step  $\frac{1}{n}$  and space step  $\frac{1}{\sqrt{n}}$ .

## 1.6 Other stochastic processes

We present other one-dimensional processes, with continuous trajectories, which derive from the Brownian motion.

1. Geometric Brownian motion: this model is popular in finance to model stocks and other assets by a positive process.
2. Ornstein-Uhlenbeck process: it has important applications in physics, mechanics, economy and finance to model stochastic phenomena exhibiting mean-reverting features (like spring endowed with random forces, interest-rates or inflation, ...).
3. Stochastic differential equations: it gives the more general framework.

### 1.6.1 Geometric Brownian motion

**Definition 1.14** *A Geometric Brownian Motion (GBM in short) with deterministic initial value  $S_0 > 0$ , drift coefficient  $\mu$  and diffusion coefficient  $\sigma$ , is a process  $(S_t)_{t \geq 0}$  defined*



by

$$S_t = S_0 e^{(\mu - \frac{1}{2}\sigma^2)t + \sigma W_t}, \quad (1.9)$$

where  $\{W_t; t \geq 0\}$  is standard BM.

As the argument in the exponential has a Gaussian distribution, the random variable  $S_t$  (with  $t$  fixed) is known as Lognormal.

This is a process with continuous trajectories, which takes strictly positive values. The GBM is often used as a model of asset (see Samuelson [Sam65]): this choice is justified on the one hand, by the positivity of  $S$  and on the other hand, by the simple Gaussian properties of its returns:

- the returns  $\log(S_t) - \log(S_s)$  are Gaussian with mean  $(\mu - \frac{1}{2}\sigma^2)(t - s)$  and variance  $\sigma^2(t - s)$ .
- For all  $0 < t_1 < t_2 \dots < t_n$ , the relative increments  $\{\frac{S_{t_{i+1}}}{S_{t_i}}; 0 \leq i \leq n - 1\}$  are independent.

The assumption of Gaussian returns is not valid in practice but this model still serves as a proxy for more sophisticated model.

Naming  $\mu$  the drift parameter may be surprising at first sight since it appears in the deterministic component as  $(\mu - \frac{1}{2}\sigma^2)t$ . Actually, a computation of expectation gives easily

$$\mathbb{E}(S_t) = S_0 e^{(\mu - \frac{1}{2}\sigma^2)t} \mathbb{E}(e^{\sigma W_t}) = S_0 e^{(\mu - \frac{1}{2}\sigma^2)t} e^{\frac{1}{2}\sigma^2 t} = S_0 e^{\mu t}.$$

The above equality gives the interpretation to  $\mu$  as a mean drift term:  $\mu = \frac{1}{t} \log[\mathbb{E}(S_t)/S_0]$ .

### 1.6.2 Ornstein-Uhlenbeck process

Let us return to physics and to the Brownian motion by Einstein in 1905. In order to propose a more adequate modeling of the phenomenon of particles diffusion, we introduce the process of Ornstein-Uhlenbeck and its principal properties.

So far we have built the Brownian motion like a model for a microscopic particle in suspension in a liquid subjected to thermal agitation. An important criticism made with this modeling concerns the assumption that displacement increments are independent and they do not take into account the effects of the particle speed due to particle inertia.

Let us denote by  $m$  the particle mass and by  $\dot{X}(t)$  its speed. Owing to Newton's second law, the momentum change  $m\dot{X}(t + \delta(t)) - m\dot{X}(t)$  is equal to the resistance  $-k\dot{X}(t)\delta t$  of the medium during time  $\delta t$ , plus the momentum change due to molecular shocks, that we assume to be with stationary independent increments and thus associated with a BM. The process thus modeled is called sometimes the *physical Brownian motion*. The equation for the increments becomes

$$m \delta[\dot{X}(t)] = -k\dot{X}(t)\delta t + m\sigma\delta W_t.$$

Trajectories of the Brownian motion being not differentiable, the equation has to be read in an integral form

$$m\dot{X}(t) = m\dot{X}(0) + \int_0^t -k\dot{X}(s)ds + m\sigma W_t.$$

$\dot{X}(t)$  is thus solution of the linear stochastic differential equation (known as Langevin equation)

$$V_t = v_0 - a \int_0^t V_s ds + \sigma W_t$$

where  $a = \frac{k}{m}$ . If  $a = 0$ , we recover an arithmetic BM and to avoid this reduction, we assume  $a \neq 0$  in the sequel. However, the existence of solution is not clear since  $W$  is

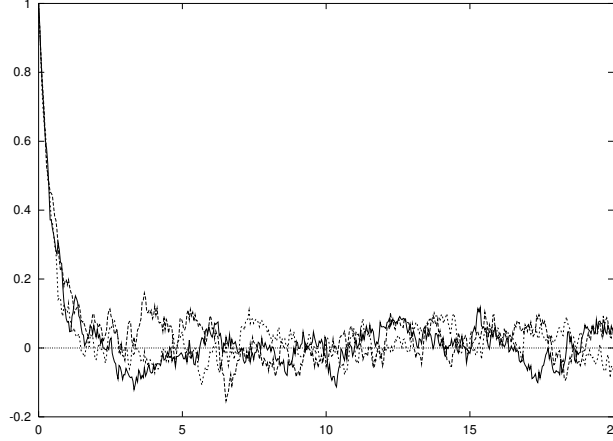


Figure 1.5: Ornstein-Uhlenbeck paths with  $V_0 = 1$ ,  $a = 2$  and  $\sigma = 0.1$ .

not differentiable. To overcome this difficulty, set  $Z_t = V_t - \sigma W_t$ : that leads to the new equation

$$Z_t = v_0 - a \int_0^t (Z_s + \sigma W_s) ds,$$

which is now a linear ordinary differential equation that can be solved path by path. The variation of parameter method gives the representation of the unique solution of this equation like

$$Z_t = v_0 e^{-at} - \sigma \int_0^t a e^{-a(t-s)} W_s ds.$$

The initial solution is thus

$$V_t = v_0 e^{-at} + \sigma W_t - \sigma \int_0^t a e^{-a(t-s)} W_s ds. \quad (1.10)$$

Using stochastic calculus, we will derive later (see Subsection 3.3) another convenient representation of  $V$  as follows:

$$V_t = v_0 e^{-at} + \sigma \int_0^t e^{-a(t-s)} dW_s \quad (1.11)$$

using a stochastic integral not yet defined. From (1.10), assuming that  $v_0$  is deterministic, we can show the following properties (see also Subsection 3.3).

- For a given  $t$ ,  $V_t$  has a Gaussian distribution: indeed, as the limit of a Riemann sum, it is the *a.s.* limit a Gaussian r.v, see footnote 6 page 7.

- More generally,  $V$  is a Gaussian process.
- Its mean is  $v_0 e^{-at}$ , its covariance function  $\text{Cov}(V_t, V_s) = e^{-a(t-s)} \frac{\sigma^2}{2a} (1 - e^{-2at})$  for  $t > s$ .

Observe that for  $a > 0$ , the Gaussian distribution parameters of  $V_t$  converges to  $\mathcal{N}(0, \frac{\sigma^2}{2a})$  as  $t \rightarrow +\infty$ : it does not depend anymore on  $v_0$  and illustrates the mean-reverting feature of this model, see Figure 1.5.

### 1.6.3 Stochastic differential equations and Euler approximations

The previous example gives the generic form of a Stochastic Differential Equation, that generalizes the usual Ordinary Differential Equations  $x'_t = b(x_t)$  or in integral form  $x_t = x_0 + \int_0^t b(x_s) ds$ .

**Definition 1.15** *Let  $b, \sigma : x \in \mathbb{R} \mapsto \mathbb{R}$  be two functions, respectively the drift and the diffusion coefficient. A Stochastic Differential Equation (SDE in short) with parameter  $(b, \sigma)$  and initial value  $x$  is a stochastic process  $(X_t)_{t \geq 0}$  solution of*

$$X_t = x + \int_0^t b(X_s) ds + \int_0^t \sigma(X_s) dW_s, \quad t \geq 0,$$

where  $(W_t)_t$  is a standard BM.

In this definition, we use a stochastic integral  $\int_0^t \dots dW_s$  which has not yet been defined: it will be explained in the next section. For the moment, the reader needs to know that in the simplest case where  $\sigma$  is constant, we simply have  $\int_0^t \sigma(X_s) dW_s = \sigma W_t$ . The previous examples fit this setting:

- the arithmetic BM corresponds to  $b(t, x) = b$  et  $\sigma(t, x) = \sigma$ ;
- the OU process corresponds to  $b(t, x) = -ax$  et  $\sigma(t, x) = \sigma$ .

Taking  $\sigma$  to be non constant allows for more general situations and more flexible models. Instead of discussing now the important issues of existence and uniqueness to such SDE, we rather consider natural approximations of them, namely the Euler scheme (which is the direct extension of Euler scheme for ODEs).

**Definition 1.16** *Let  $(b, \sigma)$  be given drift and diffusion coefficients. The Euler scheme associated to the SDE with coefficients  $(b, \sigma)$ , initial value  $x$  and time step  $h$ , is defined by*

$$\begin{cases} X_0^h = x, \\ X_t^h = X_{ih}^h + b(X_{ih}^h)(t - ih) + \sigma(X_{ih}^h)(W_t - W_{ih}), \quad i \geq 0, \quad t \in (ih, (i+1)h]. \end{cases} \quad (1.12)$$

In other words,  $X^h$  is a piecewise arithmetic BM with coefficients on the interval  $(ih, (i+1)h]$  computed according to the functions  $(b, \sigma)$  evaluated at  $X_{ih}^h$ . In general, the law of  $X_t^h$  is not known analytically: at most, we can give explicit representations using an induction of the time-step. On the other hand, as it will be seen further, the random simulation of  $X^h$  at time  $(ih)_{i \geq 0}$  is easily performed by simulating the independent Brownian increments  $(W_{(i+1)h} - W_{ih})$ . The accuracy of the approximation of  $X$  by  $X^h$  is expected to get improved as  $h$  goes to 0.

**Complementary references:** see [Nel67], [KS91], [RY05].

## 2 Feynman-Kac representations of PDE solutions

Our purpose in this section is to make the connection between the expectations of functionals of BM and the solution of second order linear parabolic partial differential equations (PDE in short): this leads to the well-known Feynman-Kac representations. We extend this point of view to other simple processes introduced before.

### 2.1 The heat equations

#### 2.1.1 Heat equation in the whole space

Let us return to the law of  $x + W_t$  which Gaussian density is

$$g(t, x, y) := g(t, y - x) = \frac{1}{\sqrt{2\pi t}} \exp(-(y - x)^2/2t),$$

often called in this context the fundamental solution of the heat equation. One of the key properties is *the property of convolution*

$$g(t + s, x, y) = \int_{\mathbb{R}} g(t, x, z)g(s, z, y)dz \quad (2.1)$$

which says in an analytical language that  $x + W_{t+s}$  is the sum of the independent Gaussian variables  $x + W_t$  and  $W_{t+s} - W_t$ . A direct calculation on the density shows that the Gaussian density is solution to the *heat equation* w.r.t. the two variables  $x$  and  $y$

$$\begin{cases} g'_t(t, x, y) = \frac{1}{2}g''_{yy}(t, x, y), \\ g'_t(t, x, y) = \frac{1}{2}g''_{xx}(t, x, y). \end{cases} \quad (2.2)$$

This property is extended to a large class of functions built from the Brownian motion.

**Theorem 2.1 (Heat equation with Cauchy initial boundary condition)** *Let  $f$  be a bounded<sup>7</sup> measurable function. Consider the function*

$$u(t, x, f) = \mathbb{E}[f(x + W_t)] = \int_{\mathbb{R}} g(t, x, y)f(y)dy :$$

*the function  $u$  is infinitely continuously differentiable in space and time for  $t > 0$  and solves the heat equation*

$$u'_t(t, x, f) = \frac{1}{2}u''_{xx}(t, x, f), \quad u(0, x, f) = f(x). \quad (2.3)$$

---

<sup>7</sup>This growth condition can be relaxed into  $|f(x)| \leq C \exp\left(\frac{|x|^2}{2\alpha}\right)$  for any  $x$ , for some positive constants  $C$  and  $\alpha$ : in that case, the smoothness of the function  $u$  is satisfied for  $t < \alpha$  only.

Equation (2.3) is the *heat equation with initial boundary condition* (Cauchy problem, see [Fri75]).

PROOF :

Standard Gaussian estimates allow to differentiate  $u$  w.r.t.  $t$  or  $x$  by differentiating under the integral sign: then, we have

$$u'_t(t, x, f) = \int_{\mathbb{R}} g'_t(t, x, y) f(y) dy = \int_{\mathbb{R}} \frac{1}{2} g''_{xx}(t, x, y) f(y) dy = \frac{1}{2} u''_{xx}(t, x, f).$$

□

When the function considered is regular, another formulation can be given to this relation, which will play a significant role in the following.

**Proposition 2.2** *If  $f$  is of class  $\mathcal{C}_b^2$  (bounded and twice continuously differentiable with bounded derivatives)<sup>8</sup>, we have*

$$u'_t(t, x, f) = u(t, x, \frac{1}{2} f''_{xx}),$$

or equivalently using a probabilistic viewpoint

$$\mathbb{E}[f(x + W_t)] = f(x) + \int_0^t \mathbb{E}\left[\frac{1}{2} f''_{xx}(x + W_s)\right] ds. \quad (2.4)$$

PROOF :

Write  $u(t, x, f) = \mathbb{E}[f(x + W_t)] = \int_{\mathbb{R}} g(t, 0, y) f(x + y) dy = \int_{\mathbb{R}} g(t, x, z) f(z) dz$  and differentiate under the integral sign: it gives

$$\begin{aligned} u''_{xx}(t, x, f) &= \int_{\mathbb{R}} g(t, 0, y) f''_{xx}(t, x + y) dy = u(t, x, f''_{xx}) = \int_{\mathbb{R}} g''_{xx}(t, x, z) f(z) dz, \\ u'_t(t, x, f) &= \int_{\mathbb{R}} g'_t(t, x, z) f(z) dz = \frac{1}{2} \int_{\mathbb{R}} g''_{xx}(t, x, z) f(z) dz = \frac{1}{2} u(t, x, f''_{xx}), \end{aligned}$$

using at the first equality two integration by parts and at the second equality the heat equation satisfied by  $g$ . Then the probabilistic representation (2.4) easily follows:

$$\begin{aligned} \mathbb{E}[f(x + W_t)] - f(x) &= u(t, x, f) - u(0, x, f) = \int_0^t u'_t(s, x, f) ds \\ &= \int_0^t u(s, x, \frac{1}{2} f''_{xx}) ds = \int_0^t \mathbb{E}\left[\frac{1}{2} f''_{xx}(x + W_s)\right] ds. \end{aligned}$$

□

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<sup>8</sup>Here again, the boundedness could be relaxed to some exponential growth.

### 2.1.2 Heat equation in an interval

We now extend the previous results in two directions: first, we allow the function  $f$  to also depend smoothly on time and second, the final time  $t$  is replaced by a stopping time  $U$ . The first extension is straightforward and we state it without proof.

**Proposition 2.3** *Let  $f$  be a function of class  $\mathcal{C}_b^{1,2}$  (bounded, once continuously differentiable in time, twice in space, with bounded derivatives): we have*

$$\begin{aligned}\mathbb{E}[f(t, x + W_t)] &= f(0, x) + \int_0^t \mathbb{E}[f'_t(s, x + W_s) + \frac{1}{2}f''_{xx}(s, x + W_s)]ds \\ &= f(0, x) + \mathbb{E} \left[ \int_0^t (f'_t(s, x + W_s) + \frac{1}{2}f''_{xx}(s, x + W_s))ds \right]\end{aligned}\quad (2.5)$$

The second equality readily follows from Fubini's theorem to invert  $\mathbb{E}$  and time integral: this second form is more suitable for an extension to stochastic times  $t$ .

**Theorem 2.4** *Let  $f$  be a function of class  $\mathcal{C}_b^{1,2}$ , we have*

$$\mathbb{E}[f(U, x + W_U)] = f(0, x) + \mathbb{E} \left[ \int_0^U (f'_t(s, x + W_s) + \frac{1}{2}f''_{xx}(s, x + W_s))ds \right] \quad (2.6)$$

for any bounded<sup>9</sup> stopping time  $U$ .

The above identity between expectations is far to be obvious to establish by hand since the law of  $U$  is quite general and an analytical computation is out of reach. This level of generality on  $U$  is quite interesting for applications: it provides a powerful tool to determine the distribution of hitting times, to show how often multidimensional BM visits a given point or a given set. Regarding this lecture, it gives a key tool to derive probabilistic representations of heat equation with Dirichlet boundary conditions.

PROOF :

Let us start by giving alternatives of the relation (2.5). We observe that it could have been written with a random initial condition  $X_0$ , like for instance

$$\mathbb{E}[\mathbf{1}_{A_0}f(t, X_0 + W_t)] = \mathbb{E} \left[ \mathbf{1}_{A_0}f(0, X_0) + \mathbf{1}_{A_0} \int_0^t (f'_t(s, X_0 + W_s) + \frac{1}{2}f''_{xx}(s, X_0 + W_s))ds \right],$$

with  $W$  independent of  $X_0$  and where the event  $A_0$  depends on  $X_0$ . Similarly, using the time-shifted BM  $\{\bar{W}_t^u = W_{t+u} - W_u; t \in \mathbb{R}^+\}$  that is independent of the initial condition  $x + W_u$  (Proposition 1.5), it leads to

$$\begin{aligned}\mathbb{E}[\mathbf{1}_{A_u}f(t+u, x + W_u + \bar{W}_t^u)] &= \mathbb{E} \left[ \mathbf{1}_{A_u}f(u, x + W_u) + \right. \\ &\quad \left. \mathbf{1}_{A_u} \int_0^t (f'_t(u+s, x + W_u + \bar{W}_s^u) + \frac{1}{2}f''_{xx}(u+s, x + W_u + \bar{W}_s^u))ds \right]\end{aligned}$$

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<sup>9</sup>meaning that for a deterministic positive constant  $C$ ,  $\mathbb{P}(U \leq C) = 1$

for any event  $A_u$  depending only of the values  $\{W_s : s \leq u\}$ , or equivalently

$$\begin{aligned} \mathbb{E}[\mathbf{1}_{A_u} f(t+u, x+W_{t+u})] = & \mathbb{E} \left[ \mathbf{1}_{A_u} f(u, x+W_u) \right. \\ & \left. + \mathbf{1}_{A_u} \int_u^{t+u} (f'_t(s, x+W_s) + \frac{1}{2} f''_{xx}(s, x+W_s)) ds \right]. \end{aligned}$$

Set  $M_t = f(t, x+W_t) - f(0, x) - \int_0^t (f'_t(s, x+W_s) + \frac{1}{2} f''_{xx}(s, x+W_s)) ds$ : our aim is to prove  $\mathbb{E}(M_U) = 0$ . Observe that the preliminary computation has shown that

$$\mathbb{E}(\mathbf{1}_{A_u}(M_{t+u} - M_u)) = 0 \quad (2.7)$$

for  $t \geq 0$ . In particular, taking  $A_u = \Omega$  we obtain that the expectation  $\mathbb{E}(M_t)$  is constant<sup>10</sup> w.r.t.  $t$ .

Now, consider first that  $U$  is a discrete stopping time valued in  $\{0 = u_0 < u_1 < \dots < u_n = T\}$ : then

$$\mathbb{E}(M_U) = \sum_{k=0}^{n-1} \mathbb{E}(M_{U \wedge u_{k+1}} - M_{U \wedge u_k}) = \sum_{k=0}^{n-1} \mathbb{E}(\mathbf{1}_{U > u_k}(M_{u_{k+1}} - M_{u_k})) = 0$$

by applying (2.7) since  $\{U \leq u_k\}$  does depend only of  $\{W_s : s \leq u_k\}$  (by definition of a stopping time).

Second, for a general stopping time (bounded by  $T$ ), we take  $U_n = \frac{[nU]+1}{n}$  which is a stopping time converging to  $U$ : since  $(M_t)_{0 \leq t \leq T}$  is bounded and continuous, the dominated convergence theorem gives  $0 = \mathbb{E}(M_{U_n}) \xrightarrow{n \rightarrow \infty} \mathbb{E}(M_U)$ .  $\square$

As a consequence, we now make explicit the solutions of the heat equation in an interval and with initial condition: it is a partial generalization<sup>11</sup> of Theorem 2.1, which characterized them in the whole space. The introduction of (non-homogeneous) boundary conditions of Dirichlet type is connected to the passage time of the Brownian motion.

**Corollary 2.5 (Heat equation with Cauchy-Dirichlet boundary condition)** *Consider the PDE*

$$\begin{cases} u'_t(t, x) = \frac{1}{2} u''_{xx}(t, x), & \text{for } t > 0 \text{ and } x \in ]a, b[, \\ u(0, x) = f(0, x) & \text{for } t = 0 \text{ and } x \in [a, b], \\ u(t, x) = f(t, x) & \text{for } x = a \text{ or } b, \text{ with } t \geq 0. \end{cases}$$

*If a solution  $u$  of class  $C_b^{1,2}([0, T] \times [a, b])$  exists, then it is given by*

$$u(t, x) = \mathbb{E}[f(t - U, x + W_U)]$$

*where  $U = T_a \wedge T_b \wedge t$  (using the previous notation for the first passage time  $T_y$  at the level  $y$  for the BM starting at  $x$  (i.e.  $(x + W_t)_{t \geq 0}$ ).*

<sup>10</sup>actually, (2.7) proves that  $M$  is a martingale and the result to be proved is related to the *optional sampling theorem*.

<sup>11</sup>indeed, the result gives uniqueness and not the existence.

PROOF :

First, extend smoothly the function  $u$  outside the interval  $[a, b]$  in order to apply previous results. The way to extend is unimportant since  $u$  and its derivatives are only evaluated inside  $[a, b]$ . Clearly  $U$  is a bounded (by  $t$ ) stopping time. Apply now the equality (2.6) to the function  $(s, y) \mapsto u(t - s, y) = v(s, y)$  of class  $C_b^{1,2}([0, t] \times \mathbb{R})$ , satisfying  $v'_s(s, y) + \frac{1}{2}v''_{yy}(s, y) = 0$  for  $(s, y) \in [0, t] \times [a, b]$ . We obtain

$$\mathbb{E}[v(U, x + W_U)] = v(0, x) + \mathbb{E} \left[ \int_0^U (v'_s(s, x + W_s) + \frac{1}{2}v''_{yy}(s, x + W_s)) ds \right] = v(0, x),$$

since for  $s \leq U$ ,  $(s, x + W_s) \in [0, t] \times [a, b]$ . To conclude, we easily check that  $v(0, x) = u(t, x)$  and  $v(U, x + W_U) = f(t - U, x + W_U)$ .  $\square$

### 2.1.3 A probabilistic algorithm to solve the heat equation

To illustrate our purpose, we consider a toy example regarding the numerical evaluation of  $u(t, x) = \mathbb{E}(f(x + W_t))$  using random simulations, in order to discuss main ideas underlying to Monte Carlo methods. Actually, the arguments below apply also to  $u(t, x) = \mathbb{E}[f(t - U, x + W_U)]$  with  $U = T_a \wedge T_b \wedge t$ , although there are some extra significant issues in the simulation of  $(U, W_U)$ .

For the notational simplicity, denote by  $X$  the random variable inside the expectation to compute, that is  $X = f(x + W_t)$  in our toy example. As a difference with a PDE method (based on finite differences of finite elements), a standard Monte Carlo method provides an approximation of  $u(t, x)$  at a given point  $(t, x)$ , without evaluating the values at other points. Actually, this fact holds because the PDE  $u$  is linear; in Section 5 related to non-linear PDEs, the situation is different.

The Monte Carlo method is able to provide a convergent, tractable approximation of  $u(t, x)$ , with a priori error bounds, under two conditions.

1. An arbitrary large number of independent realizations of  $X$  can be generated (denote them by  $(X_i)_{i \geq 1}$ ): in our toy example, this is straightforward since it requires only the simulation of  $W_t$  which is distributed as a Gaussian r.v.  $\mathcal{N}(0, t)$  and then we have to compute  $X = f(x + W_t)$ . The independence of simulations is achieved by using a *good* generator of random numbers, like the *Mersenne Twister*<sup>12</sup> generator.
2. Additionally,  $X$  which is already integrable ( $\mathbb{E}|X| < +\infty$ ) is assumed to be square integrable:  $\text{Var}(X) < +\infty$ .

Then, by the law of large numbers, we have

$$\bar{X}_M = \frac{1}{M} \sum_{i=1}^M X_i \xrightarrow{M \rightarrow +\infty} \mathbb{E}(X); \quad (2.8)$$

hence the empirical mean of simulations of  $X$  provides a convergent approximation of the expectation  $\mathbb{E}(X)$ . As a difference with PDE methods where some stability conditions may

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<sup>12</sup><http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html>



be required (like the Courant-Friedrichs-Lewy condition), the above Monte Carlo method does not require any extra condition to converge: it is *unconditionally convergent*. The extra moment condition is used to define a priori error bounds on the *statistical error*: the approximation error is controlled by means of the Central Limit Theorem

$$\lim_{M \rightarrow +\infty} \mathbb{P} \left( \sqrt{\frac{M}{\mathbb{V}\text{ar}(X)}} (\bar{X}_M - \mathbb{E}(X)) \in [a, b] \right) = \mathbb{P}(G \in [a, b]),$$

where  $G$  is a centered unit variance Gaussian r.v. Observe that the error bounds are stochastic: we can not do better than arguing that with probability  $\mathbb{P}(G \in [a, b])$ , the unknown expectation (asymptotically as  $M \rightarrow +\infty$ ) belongs to the interval

$$\left[ \bar{X}_M - b \sqrt{\frac{\mathbb{V}\text{ar}(X)}{M}}, \bar{X}_M - a \sqrt{\frac{\mathbb{V}\text{ar}(X)}{M}} \right].$$

This is known as a confidence interval at level  $\mathbb{P}(G \in [a, b])$ . The larger  $a$  and  $b$ , the larger the confidence interval, the higher the confidence probability.

To obtain a fully explicit confidence interval, one may replace  $\mathbb{V}\text{ar}(X)$  by its evaluation using the same simulations:

$$\mathbb{V}\text{ar}(X) = \mathbb{E}(X^2) - (\mathbb{E}(X))^2 \approx \frac{M}{M-1} \left( \frac{1}{M} \sum_{i=1}^M X_i^2 - \bar{X}_M^2 \right) := \sigma_M^2.$$

The factor  $M/(M-1)$  plays the role of unbiasing<sup>13</sup> the value  $\mathbb{V}\text{ar}(X)$ , although it is not a big deal for  $M$  large ( $M \geq 100$ ). Anyway, we can prove that the above conditional intervals are asymptotically unchanged by taking the empirical variance  $\sigma_M^2$  instead of  $\mathbb{V}\text{ar}(X)$ . Gathering these different results and seeking a symmetric confidence interval  $-a = b = 1.96$  and  $\mathbb{P}(G \in [a, b]) \approx 95\%$ , we obtain the following: with probability 95%, for  $M$  large enough, we have

$$\mathbb{E}(X) \in \left[ \bar{X}_M - 1.96 \frac{\sigma_M}{\sqrt{M}}, \bar{X}_M - 1.96 \frac{\sigma_M}{\sqrt{M}} \right]. \quad (2.9)$$

The symmetric confidence interval at level 99% is given by  $-a = b = 2.58$ . Since a Monte Carlo method provides random evaluations of  $\mathbb{E}(X)$ , different program runs will give different results (as a difference with a deterministic method which systematically has the same output) which seems uncomfortable: that is why it is important to produce a confidence interval. This is also very powerful and useful to have at hand a numerical method able to state that the error is at most of xxx with high probability.

The confidence interval depends on

- the confidence level  $\mathbb{P}(G \in [a, b])$ , chosen by the user;
- the number of simulations: improving the accuracy by a factor 2 requires 4 times more simulations;

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<sup>13</sup>Indeed, we can show that  $\mathbb{E}(\sigma_M^2) = \mathbb{V}\text{ar}(X)$ .

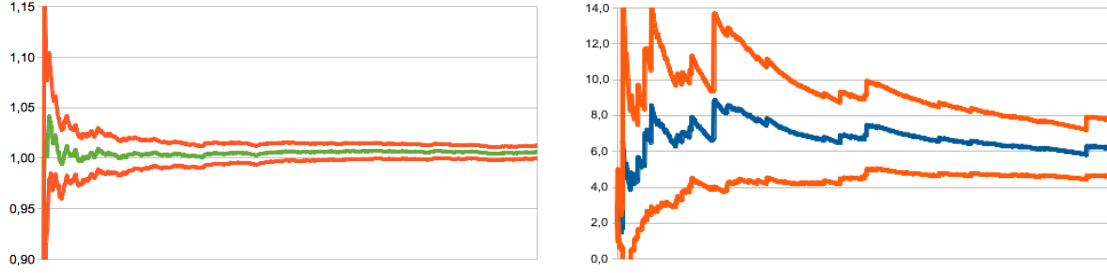


Figure 2.1: Monte Carlo computations of  $\mathbb{E}(e^{G/10}) = e^{\frac{1}{2} \frac{1}{10^2}} \approx 1.005$  on the left and  $\mathbb{E}(e^{2G}) = e^{\frac{1}{2} 2^2} \approx 7.389$  on the right, where  $G$  is a Gaussian r.v. with zero mean and unit variance. The empirical mean and the symmetric 95%-confidence intervals are plotted w.r.t. the number of simulations.

- the variance  $\text{Var}(X)$  or its numerical approximation  $\sigma_M^2$ , which depends on the problem to handle (and not much on  $M$  as soon as  $M$  is large). This variance can be very different from one problem to another: on Figure 2.1, see the width of confidence intervals for two similar computations. There exist variance reduction techniques able to significantly reduce this factor in order to provide thicker confidence intervals while maintaining the same computational cost.

Another advantage of such a Monte Carlo algorithm is the simplicity of code, consisting of one loop on the number of simulations; within this loop, the empirical variance should be simultaneously computed. However, the simulation procedure of  $X$  can be delicate in some situations, see Section 4.

At last, we focus our discussion on the impact of the dimension of the underlying PDE, which has been equal to 1 so far. Consider now a state variable in  $\mathbb{R}^d$  ( $d \geq 1$ ) and a heat equation with Cauchy initial condition in dimension  $d$ ; (2.3) becomes

$$u'_t(t, x, f) = \frac{1}{2} \Delta u(t, x, f), \quad u(0, x, f) = f(x), \quad t > 0, x \in \mathbb{R}^d, \quad (2.10)$$

where  $\Delta = \sum_{i=1}^d \partial_{x_i x_i}^2$  stands for the Laplacian in  $\mathbb{R}^d$ . Using similar arguments as in dimension 1, we check that

$$u(t, x, f) = \int_{\mathbb{R}^d} \frac{1}{(2\pi t)^{d/2}} \exp(-|y - x|^2/2t) f(y) dy = \mathbb{E}[f(x + W_t)]$$

where  $W = \begin{pmatrix} W_1 \\ \vdots \\ W_d \end{pmatrix}$  is  $d$ -dimensional BM, i.e. each  $W_i$  is one-dimensional BM and the  $d$  components are independent.

- The Monte Carlo computation of  $u(t, x)$  is then achieved using independent simulations of  $X = f(x + W_t)$ : the accuracy is then of order  $1/\sqrt{N}$  and the computational effort is  $N \times d$ . Thus, the dimension has a very low effect on the complexity of the algorithm.

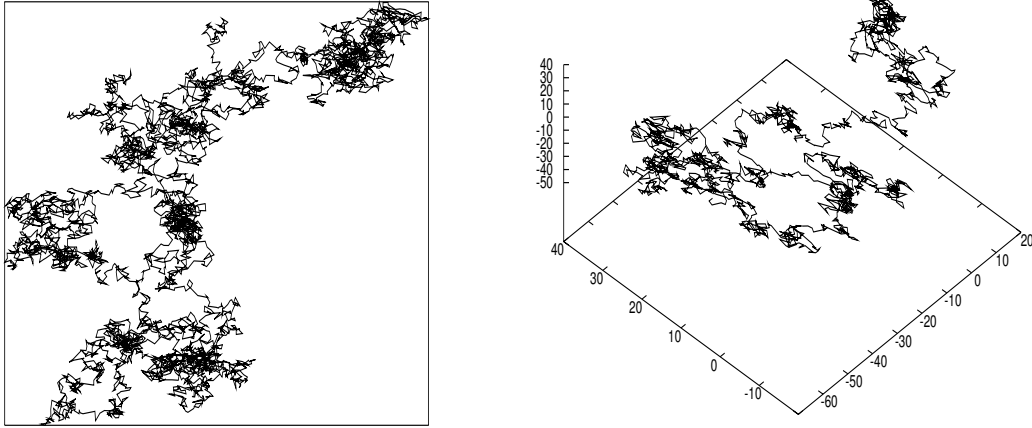


Figure 2.2: Brownian motion in dimension 2 and 3.

- As a comparison with a PDE discretization scheme, to achieve an accuracy of order  $1/N$ , we essentially<sup>14</sup> need  $N$  points in each spatial direction and it follows that the resulting linear system to invert is of size  $N^d$ : thus, without going into full details, it is clear that the computational cost to achieve a given accuracy depends much on the dimension  $d$ . And the situation becomes less and less favourable as the dimension increases. Also, the memory required to run a PDE algorithm increases exponentially with the dimension, as a difference with a Monte Carlo approach.

It is commonly admitted that a PDE approach is more suitable and efficient in dimension 1 and 2, whereas a Monte Carlo procedure is more adapted for higher dimensions. On the other hand, a PDE-based method computes a global approximation of  $u$  (at any point  $(t, x)$ ), while a Monte Carlo scheme gives a pointwise approximation only. The probabilistic approach can be directly used for Parallel Computing, each processor being in charge of a bunch of simulations at a given point  $(t, x)$ .

## 2.2 PDE associated to other processes

We extend the Feynman-Kac representation for the BM to the Arithmetic Brownian Motion and the Ornstein-Uhlenbeck process.

### 2.2.1 Arithmetic Brownian Motion

First consider the Arithmetic BM defined by  $\{X_t^x = x + bt + \sigma W_t, t \geq 0\}$ . The distribution of  $X_t$  is Gaussian with mean  $x + bt$  and variance  $\sigma^2 t$ : we assume in the following that  $\sigma \neq 0$  which ensures that its density exists and is given by

$$g_{b,\sigma^2}(t, x, y) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp - \frac{(y - x - bt)^2}{2\sigma^2 t} = g(\sigma^2 t, x + bt, y) = g(\sigma^2 t, x, y - bt).$$

<sup>14</sup>In fact, it generally depends on the regularity of  $u$ .

Denote by  $L_{b,\sigma^2}^{\text{ABM}}$  the second order operator

$$L_{b,\sigma^2}^{\text{ABM}} = \frac{1}{2}\sigma^2\partial_{xx}^2 + b\partial_x, \quad (2.11)$$

also called *infinitesimal generator*<sup>15</sup> of  $X$ . A direct computation using the heat equation for  $g(t, x, y)$  gives

$$\partial_t g_{b,\sigma^2}(t, x, y) = \frac{1}{2}\sigma^2 g_{xx}''(\sigma^2 t, x + bt, y) + b g_x'(\sigma^2 t, x + bt, y) = L_{b,\sigma^2}^{\text{ABM}} g_{b,\sigma^2}(t, x, y).$$

Hence, multiplying by  $f(y)$  and integrating over  $y \in \mathbb{R}$ , we obtain the following representation that generalizes Theorem 2.1.

**Theorem 2.6** *Let  $f$  be a bounded measurable function. The function*

$$u_{b,\sigma^2}(t, x, f) = \mathbb{E}[f(X_t^x)] = \int_{\mathbb{R}} g_{b,\sigma^2}(t, x, y) f(y) dy \quad (2.12)$$

*solves*

$$\begin{cases} u_t'(t, x, f) = L_{b,\sigma^2}^{\text{ABM}} u(t, x, f) = \frac{1}{2}\sigma^2 u_{xx}''(t, x, f) + b u_x'(t, x, f), \\ u(0, x, f) = f(x). \end{cases} \quad (2.13)$$

The extension of Propositions 2.2 and 2.3 follows the arguments used for the BM case.

**Proposition 2.7** *If  $f \in \mathcal{C}_b^{1,2}$  and  $U$  is a bounded stopping time (including deterministic time), then  $\mathbb{E}[f(U, X_U^x)] = f(0, x) + \mathbb{E}\left[\int_0^U [L_{b,\sigma^2}^{\text{ABM}} f(s, X_s^x) + f_t'(s, X_s^x)] ds\right]$ .*

Theorem 2.6 gives the Feynman-Kac representation of the Cauchy problem written w.r.t. the second order operator  $L_{b,\sigma^2}^{\text{ABM}}$ . When Dirichlet boundary conditions are added, Corollary 2.5 extends as follows, using Proposition 2.7.

**Corollary 2.8** *Assume the existence of a solution  $u$  of class  $C_b^{1,2}([0, T] \times [a, b])$  to the PDE*

$$\begin{cases} u_t'(t, x, f) = L_{b,\sigma^2}^{\text{ABM}} u(t, x, f), & \text{for } t > 0 \text{ and } x \in ]a, b[, \\ u(0, x, f) = f(0, x) & \text{for } t = 0 \text{ and } x \in [a, b], \\ u(t, x, f) = f(t, x) & \text{for } x = a \text{ or } b, \text{ with } t \geq 0. \end{cases}$$

*Then it is given by*

$$u(t, x) = \mathbb{E}[f(t - U^x, X_{U^x}^x)]$$

*where  $U^x = \inf\{s > 0 : X_s^x \notin ]a, b[ \} \wedge t$  is the exit time from the interval  $]a, b[$  by the process  $X^x$  before  $t$ .*

As for the standard heat equation, this representation naturally leads to a probabilistic algorithm to compute the PDE solution, by empirical mean of independent simulation of  $f(t - U^x, X_{U^x}^x)$ .

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<sup>15</sup>This labeling comes from the infinitesimal decomposition of  $\mathbb{E}(f(X_t))$  as time is small,  $\partial_t \mathbb{E}(f(X_t))|_{t=0} = L_{b,\sigma^2}^{\text{ABM}} f(x)$ , see Proposition 2.7.

### 2.2.2 Ornstein-Uhlenbeck process

Now consider the process solution to  $V_t^x = x - a \int_0^t V_s^x ds + \sigma W_t$ : we emphasize in our notation the dependence w.r.t. the initial value  $V_0 = x$ . We define an appropriate second order operator

$$L_{a,\sigma^2}^{\text{OU}} g(t, x) = \frac{1}{2} \sigma^2 g''_{xx}(t, x) - ax g'_x(t, x)$$

which plays the role of the infinitesimal generator for the OU process. We recall that the Gaussian distribution of  $V_t^x$  has mean  $x e^{-at}$  and variance  $\frac{\sigma^2}{2a}(1 - e^{-2at})$ , which density at  $y$  (assuming  $\sigma \neq 0$  for the existence) is

$$p(t, x, y) = g(v_t, x e^{-at}, y).$$

Using the heat equation satisfied by  $g$ , we easily derive that

$$p'_t(t, x, y) = \frac{1}{2} \sigma^2 p''_{xx}(t, x, y) - ax p'_x(t, x, y) = L_{a,\sigma^2}^{\text{OU}} p(t, x, y),$$

from which we deduce the PDE satisfied by  $u(t, x, f) = \mathbb{E}[f(V_t^x)]$ . Incorporating Dirichlet boundary conditions is similar to the previous cases. We state the related results without extra details.

**Theorem 2.9** *Let  $f$  be a bounded measurable function. The function*

$$u(t, x, f) = \mathbb{E}[f(V_t^x)] = \int_{\mathbb{R}} p(t, x, y) f(y) dy$$

*solves*

$$\begin{cases} u'_t(t, x, f) = L_{a,\sigma^2}^{\text{OU}} u(t, x, f), \\ u(0, x, f) = f(x). \end{cases}$$

**Proposition 2.10** *If  $f \in \mathcal{C}_b^{1,2}$  and  $U$  is a bounded stopping time, then  $\mathbb{E}[f(U, V_U^x)] = f(0, x) + \mathbb{E}\left[\int_0^U [L_{a,\sigma^2}^{\text{OU}} f(s, V_s^x) + f'_t(s, V_s^x)] ds\right]$ .*

**Corollary 2.11** *Assume the existence of a solution  $u$  of class  $C_b^{1,2}([0, T] \times [a, b])$  to the PDE*

$$\begin{cases} u'_t(t, x, f) = L_{a,\sigma^2}^{\text{OU}} u(t, x, f), & \text{for } t > 0 \text{ and } x \in ]a, b[, \\ u(0, x, f) = f(0, x) & \text{for } t = 0 \text{ and } x \in [a, b], \\ u(t, x, f) = f(t, x) & \text{for } x = a \text{ or } b, \text{ with } t \geq 0. \end{cases}$$

*Then it is given by*

$$u(t, x) = \mathbb{E}[f(t - U^x, V_{U^x}^x)]$$

*where  $U^x = \inf\{s > 0 : V_s^x \notin ]a, b[ \} \wedge t$ .*

### 2.2.3 A natural conjecture for Stochastic Differential Equations

The previous examples serve as a preparation for more general results, relating the dynamics of a process and its Feynman-Kac representation. Denote  $X^x$  the solution (whenever it exists) to the Stochastic Differential Equation

$$X_t^x = x + \int_0^t b(X_s^x)ds + \int_0^t \sigma(X_s^x)dW_s, \quad t \geq 0.$$

In view of the results in simpler models, we announce the following facts.

1. Set  $L_{b,\sigma^2}^X g = \frac{1}{2}\sigma^2(x)g''_{xx} + b(x)g'_x$ .
2.  $u(t, x) = \mathbb{E}(f(X_t^x))$  solves

$$u'_t(t, x) = L_{b,\sigma^2}^X u(t, x), \quad u(0, x) = f(x).$$

3. If  $f \in C_b^{1,2}$  and  $U$  is a bounded stopping time, then  $\mathbb{E}[f(U, X_U^x)] = f(0, x) + \mathbb{E}\left[\int_0^U [L_{b,\sigma^2}^X f(s, X_s^x) + f'_t(s, X_s^x)]ds\right]$ .
4. If  $u$  of class  $C_b^{1,2}([0, T] \times [a, b])$  solves the PDE

$$\begin{cases} u'_t(t, x) = L_{b,\sigma^2}^X u(t, x), & \text{for } t > 0 \text{ and } x \in ]a, b[, \\ u(0, x) = f(0, x) & \text{for } t = 0 \text{ and } x \in [a, b], \\ u(t, x) = f(t, x) & \text{for } x = a \text{ or } b, \text{ with } t \geq 0, \end{cases}$$

then it is given by  $u(t, x) = \mathbb{E}[f(t - U^x, X_{U^x}^x)]$  where  $U^x = \inf\{s > 0 : X_s^x \notin ]a, b[ \} \wedge t$ .

The above result could be extended to PDE with a space variable in  $\mathbb{R}^d$  ( $d \geq 1$ ) by considering a  $\mathbb{R}^d$ -valued SDE: it would be achieved by replacing  $W$  by a  $d$ -dimensional standard Brownian motion, by having a drift coefficient  $b : \mathbb{R}^d \mapsto \mathbb{R}^d$  and a diffusion coefficient  $\sigma : \mathbb{R}^d \mapsto \mathbb{R}^d \otimes \mathbb{R}^d$ , a reward function  $f : [0, T] \times \mathbb{R}^d \mapsto \mathbb{R}$ , by replacing the interval  $[a, b]$  by a domain  $D$  in  $\mathbb{R}^d$  and defining  $U^x$  as the first exit time by  $X^x$  from that domain. Then the operator  $L$  would be a linear parabolic second order operator of the form

$$L_{b,\sigma\sigma^\perp}^X g = \frac{1}{2} \sum_{i,j=1}^d [\sigma\sigma^\perp]_{i,j}(x) \partial_{x_i x_j}^2 g + \sum_{i=1}^d b_i(x) \partial_{x_i} g.$$

We could also add a zero-order term in  $L_{b,\sigma\sigma^\perp}^X$ , by considering a discounting factor for  $f$ ; we do not develop further this extension.

The next section provides stochastic calculus tools, that allow to show the validity of these Feynman-Kac type results, under some appropriate smoothness and growth assumptions on  $b, \sigma, f$ . To allow non smooth  $f$  or Dirichlet boundary conditions, we may additionally assume a non-degeneracy condition on  $L_{b,\sigma\sigma^\perp}^X$  (like ellipticity condition  $|\sigma\sigma^\top(x)| \geq \frac{1}{c}$  for some  $c > 0$ ).

**Complementary references:** see [Fri75], [Fri76], [Dur84], [Fre85], [KS91], [AP05].

### 3 The Itô formula

One achievement of Itô's formula is to go from an infinitesimal time-decomposition in expectation like

$$\mathbb{E}[f(t, x + W_t)] - f(0, x) = \int_0^t \mathbb{E}[f'_t(s, x + W_s) + \frac{1}{2}f''_{xx}(s, x + W_s)]ds$$

(see (2.5)) to a pathwise infinitesimal time-decomposition of

$$f(t, x + W_t) - f(0, x).$$

Since BM paths are not differentiable, it is hopeless to apply standard differential calculus based on usual first order Taylor formula. Instead of this, we go up to the second order, taking advantage of the fact that  $W$  has a finite quadratic variation. The approach presented below is taken from the nice paper *Calcul d'Itô sans probabilité* by Föllmer [Föl81], which does not lead to the most general and deepest approach but it has the advantage of light technicalities and straightforward arguments compared to the usual heavy arguments using  $L_2$ -spaces and isometry (see for instance [KS91] or [RY05] among others).

#### 3.1 Quadratic variation

##### 3.1.1 Notations and definitions

Brownian increments in a small interval  $[t, t+h]$  are centered Gaussian r.v. with variance  $h$ , which thus behave like  $\sqrt{h}$ . The total variation does not exist, because the trajectories are not differentiable, but the quadratic variation has interesting properties.

To avoid convergence technicalities, we consider particular time subdivisions.

**Definition 3.1 (Dyadic subdivision of order  $n$ )** *Let  $n$  be an integer. The subdivision of  $\mathbb{R}^+$  defined by  $\mathbb{D}_n = \{t_0 < \dots < t_i < \dots\}$  where  $t_i = i2^{-n}$  is called the dyadic subdivision of order  $n$ . The subdivision step is  $\delta_n = 2^{-n}$ .*

**Definition 3.2 (Quadratic variation)** *The quadratic variation of a Brownian motion  $W$  associated with the dyadic subdivision of order  $n$  is defined, for  $t \geq 0$ , by*

$$V_t^n = \sum_{t_i \leq t} (W_{t_{i+1}} - W_{t_i})^2. \quad (3.1)$$

##### 3.1.2 Convergence

Then there is the following remarkable result.

**Proposition 3.3 (Pointwise convergence)** *With probability 1, we have*

$$\lim_{n \rightarrow \infty} V_t^n = t$$

for any  $t \in \mathbb{R}^+$ .

Had  $W$  been differentiable, the limit of  $V^n$  would equal 0.

PROOF :

First let us show the *a.s.* convergence for a fixed time  $t$ , and denote by  $n(t)$  the index of the dyadic subdivision of order  $n$  such that  $t_{n(t)} \leq t < t_{n(t)+1}$ . Then observe that  $V_t^n - t = \sum_{j=0}^{n(t)} Z_j + (t_{n(t)+1} - t)$  where  $Z_j = (W_{t_{j+1}} - W_{t_j})^2 - (t_{j+1} - t_j)$ . The term  $t_{n(t)+1} - t$  converges to 0 as the subdivision step shrinks to 0. The random variables  $Z_j$  are independent, centered, square integrable (since the Gaussian law of  $W_{t_{j+1}} - W_{t_j}$  has finite fourth moments): additionally, the scaling property of Proposition 1.4 ensures that  $\mathbb{E}(Z_j^2) = C_2(t_{j+1} - t_j)^2$  for a positive constant  $C_2$ . Thus

$$\mathbb{E} \left( \sum_{j=0}^{n(t)} Z_j \right)^2 = \sum_{j=0}^{n(t)} \mathbb{E} (Z_j^2) = \sum_{j=0}^{n(t)} C_2(t_{j+1} - t_j)^2 \leq C_2(T+1)\delta_n.$$

This proves the  $L_2$ -convergence of  $\sum_{j=0}^{n(t)} Z_j$  towards 0.

Moreover we obtain  $\sum_{n \geq 1} \mathbb{E} \left( \sum_{j=0}^{n(t)} Z_j \right)^2 < \infty$ , i.e. the random series  $\sum_{n \geq 1} \left( \sum_{j=0}^{n(t)} Z_j \right)^2$  has a finite expectation, thus is *a.s.* finite and consequently its general term converges *a.s.* to 0. This shows that for any fixed  $t$ ,  $V_t^n \rightarrow t$  except on a negligible set  $N_t$ .

We now extend the result to any time: first the set  $N = \cup_{t \in \mathbb{Q}^+} N_t$  is still negligible because the union of negligible sets is taken on a countable family. For an arbitrary  $t$ , take two monotone sequences of rational numbers  $r_p \uparrow t$  and  $s_p \downarrow t$  as  $p \rightarrow +\infty$ . Since  $t \mapsto V_t^n$  is increasing for fixed  $n$ , we deduce, for any  $\omega \notin N$

$$r_p = \lim_{n \rightarrow \infty} V_{r_p}^n(\omega) \leq \liminf_{n \rightarrow \infty} V_t^n(\omega) \leq \limsup_{n \rightarrow \infty} V_t^n(\omega) \leq \lim_{n \rightarrow \infty} V_{s_p}^n(\omega) = s_p.$$

Passing to the limit in  $p$  gives the result.  $\square$

As a consequence, we obtain the formula giving the infinitesimal decomposition of  $W_t^2$ .

**Proposition 3.4 (A first Itô formula)** *Let  $W$  be a standard BM. With probability 1, we have for any  $t \geq 0$*

$$W_t^2 = 2 \int_0^t W_s dW_s + t \quad (3.2)$$

where the stochastic integral  $\int_0^t W_s dW_s$  is the *a.s.* limit of  $\sum_{t_i \leq t} W_{t_i}(W_{t_{i+1}} - W_{t_i})$ , along the dyadic subdivision.

For usual  $C^1$ -function  $f(t)$ , we have  $f^2(t) - f^2(0) = 2 \int_0^t f(s) df(s)$ : the extra term  $t$  in (3.2) is intrinsically related to BM paths.



PROOF :

Adopting once again the notation with  $n(t)$ , we have

$$\begin{aligned} W_t^2 &= W_t^2 - W_{t_{n(t)+1}}^2 + \sum_{t_i \leq t} (W_{t_{i+1}}^2 - W_{t_i}^2) \\ &= W_t^2 - W_{t_{n(t)+1}}^2 + \sum_{t_i \leq t} (W_{t_{i+1}} - W_{t_i})^2 + 2 \sum_{t_i \leq t} W_{t_i} (W_{t_{i+1}} - W_{t_i}). \end{aligned}$$

The first term at the r.h.s tends towards 0 by continuity of the Brownian paths. The second term is equal to  $V_t^n$  and converges towards  $t$ . Consequently, the third term at the right-hand side must converge *a.s.* towards a term that we call *stochastic integral* and that we denote by  $2 \int_0^t W_s dW_s$ .  $\square$

The random function  $V_t^n$ , as a function of  $t$ , is increasing and can be associated to the cumulative distribution function of the positive discrete measure

$$\sum_{i \geq 0} (W_{t_{i+1}} - W_{t_i})^2 \delta_{t_i}(\cdot) = \mu^n(\cdot)$$

satisfying  $\mu_n(f) = \sum_{i \geq 0} f(t_i) (W_{t_{i+1}} - W_{t_i})^2$ .

The convergence of cumulative distribution function of  $\mu^n(\cdot)$  (Proposition 3.3) can then be extended to integrals of continuous functions (possibly random as well). It is the purpose of the following result which is of deterministic nature.

**Proposition 3.5 (Convergence as a positive measure)** *For any continuous function  $f$ , with probability 1 we have*

$$\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f(t_i) (W_{t_{i+1}} - W_{t_i})^2 = \int_0^t f(s) ds$$

for any  $t \geq 0$ .

The proof is standard: the result first holds for functions of the form  $f(s) = \mathbf{1}_{[r_1, r_2]}(s)$ , then for piecewise constant functions, at last for continuous functions by simple approximations.

### 3.2 The Itô formula for Brownian motion

Differential calculus extends to other functions than the function  $x \rightarrow x^2$ . To the usual classical formula with functions that are smooth in time, a term should be added, due to the non-zero quadratic variation.

**Theorem 3.6 (Itô formula)** *Let  $f \in \mathcal{C}^{1,2}(\mathbb{R}^+ \times \mathbb{R}, \mathbb{R})$ . Then with probability 1, we have  $t \geq 0$*

$$\begin{aligned} f(t, x + W_t) &= f(0, x) + \int_0^t f'_x(s, x + W_s) dW_s + \int_0^t f'_t(s, x + W_s) ds \\ &\quad + \frac{1}{2} \int_0^t f''_{xx}(s, x + W_s) ds. \end{aligned} \tag{3.3}$$

The term  $\mathcal{I}_t(f) = \int_0^t f'_x(s, x + W_s) dW_s$  is called the stochastic integral of  $f'_x(s, x + W_s)$  w.r.t.  $W$  and it is the a.s. limit of

$$\mathcal{I}_t^n(f, W) = \sum_{t_i \leq t} f'_x(t_i, x + W_{t_i})(W_{t_{i+1}} - W_{t_i})$$

taken along the dyadic subdivision of order  $n$ .

The reader should compare the equality (3.3) with (2.5) to see that, under the extra assumptions that  $f$  is bounded with bounded derivatives, we have proved that the stochastic integral  $\mathcal{I}_t(f)$  is centered:

$$\mathbb{E}\left(\int_0^t f'_x(s, x + W_s) dW_s\right) = 0. \quad (3.4)$$

This explains how we can expect to go from (3.3) to (2.5):

1. apply Itô formula,
2. take expectation,
3. prove that the stochastic integral is centered.

This is an interesting alternative proof to the property satisfied by the Gaussian kernel, which is difficult to extend to more general (non Gaussian) process.

PROOF :

As before, let us introduce the index  $n(t)$  such that  $t_{n(t)} \leq t < t_{n(t)+1}$ ; then we can write

$$\begin{aligned} f(t, x + W_t) &= f(0, x) + [f(t, x + W_t) - f(t_{n(t)+1}, x + W_{t_{n(t)+1}})] \\ &\quad + \sum_{t_i \leq t} [f(t_{i+1}, x + W_{t_{i+1}}) - f(t_i, x + W_{t_{i+1}})] + \sum_{t_i \leq t} [f(t_i, x + W_{t_{i+1}}) - f(t_i, x + W_{t_i})]. \end{aligned}$$

- The second term of the r.h.s.  $[f(t, x + W_t) - f(t_{n(t)+1}, x + W_{t_{n(t)+1}})]$  converges to 0 by continuity of  $f(t, x + W_t)$ .
- The third term is analyzed by means of the first order Taylor formula:

$$f(t_{i+1}, x + W_{t_{i+1}}) - f(t_i, x + W_{t_{i+1}}) = f'_t(\tau_i, x + W_{t_{i+1}})(t_{i+1} - t_i)$$

for  $\tau_i \in ]t_i, t_{i+1}[$ . The uniform continuity of  $(W_s)_{0 \leq s \leq t+1}$  ensures that  $\sup_i |f'_t(\tau_i, x + W_{t_{i+1}}) - f'_t(t_i, x + W_{t_i})| \rightarrow 0$ : thus  $\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f'_t(\tau_i, x + W_{t_{i+1}})(t_{i+1} - t_i)$  equals to

$$\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f'_t(t_i, x + W_{t_i})(t_{i+1} - t_i) = \int_0^t f'_t(s, x + W_s) ds.$$

- A second order Taylor formula allows to write the fourth term:  $f(t_i, x + W_{t_{i+1}}) - f(t_i, x + W_{t_i})$  equals

$$f'_x(t_i, x + W_{t_i})(W_{t_{i+1}} - W_{t_i}) + \frac{1}{2} f''_{xx}(t_i, x + \xi_i)(W_{t_{i+1}} - W_{t_i})^2$$

where  $\xi_i \in (W_{t_i}, W_{t_{i+1}})$ . Similarly to before,  $\sup_i |f''_{xx}(t_i, x + \xi_i) - f''_{xx}(t_i, x + W_{t_i})| = \epsilon_n \rightarrow 0$  and it leads to

$$\left| \sum_{t_i \leq t} (f''_{xx}(t_i, x + \xi_i) - f''_{xx}(t_i, x + W_{t_i}))(W_{t_{i+1}} - W_{t_i})^2 \right| \leq \epsilon_n V_t^n,$$

$$\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f''_{xx}(t_i, x + W_{t_i})(W_{t_{i+1}} - W_{t_i})^2 = \int_0^t f''_{xx}(s, x + W_s) ds,$$

by applying Proposition 3.5.

Observe that in spite of the non-differentiability of  $W$ ,  $\sum_{t_i \leq t} f'_x(t_i, x + W_{t_i})(W_{t_{i+1}} - W_{t_i})$  is necessarily convergent as a difference of convergent terms.  $\square$

Interestingly, we obtain a representation the random variable  $f(x + W_t)$  as a stochastic integral, in terms of the derivatives of solution  $u$  to the heat equation

$$u'_t(t, x) = \frac{1}{2} u''_{xx}(t, x), \quad u(0, x) = f(x).$$

**Corollary 3.7** *Assume that  $u \in \mathcal{C}_b^{1,2}([0, T] \times \mathbb{R})$ . We have*

$$f(x + W_T) = u(T, x) + \int_0^T u'_x(T - s, x + W_s) dW_s. \quad (3.5)$$

PROOF :

Apply the Itô formula to  $v(t, x) = u(T - t, x)$  (which satisfies  $v'_t(t, x) + \frac{1}{2} v''_{xx}(t, x) = 0$ ) at time  $T$ . This gives  $f(x + W_T) = u(0, x + W_T) = u(T, x) + \int_0^T u'_x(T - s, x + W_s) dW_s$ .  $\square$

This representation formula leads to important remarks.

- If the above stochastic integral has zero expectation (as for the examples presented before), taking the expectation shows that

$$u(T, x) = \mathbb{E}(f(x + W_T)),$$

recovering the Feynman-Kac representation of Theorem 2.1.

- Then, the above representation writes, setting  $\Psi = f(x + W_T)$ ,

$$\Psi = \mathbb{E}(\Psi) + \int_0^T h_s dW_s.$$

Actually, a similar representation theorem holds in a larger generality on the form of  $\Psi$ , since any bounded<sup>16</sup> functional of  $(W_t)_{0 \leq t \leq T}$  can be represented as its expectation plus a stochastic integral: the process  $h$  is not tractable in general, whereas here it is explicitly related to the derivative of  $u$ .

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<sup>16</sup>Integrability is the right assumption.

- Assume  $u \in \mathcal{C}_b^{1,2}([0, T] \times \mathbb{R})$  imposes that  $f \in \mathcal{C}_b^2(\mathbb{R})$  which is too strong for applications: however, the assumptions on  $u$  can be relaxed to handle bounded measurable function  $f$ , because the heat equation is immediately smoothing out the initial condition. The proof of this extension involves extra stochastic calculus technicalities that we do not develop.

### 3.3 Wiener integral

In general, it is not possible to make explicit the law of the stochastic integral  $\int_0^t f'_x(s, x + W_s) dW_s$ , except in a situation where  $f'_x(s, x) = h(s)$  is independent of  $x$  and square integrable. In that case,  $\int_0^t h(s) dW_s$  is distributed as a Gaussian r.v. The resulting stochastic integral is called *Wiener integral*. We sum up its important properties.

**Proposition 3.8 (Wiener integral and integration by parts)** *Let  $f : [0, T] \mapsto \mathbb{R}$  be a continuously differentiable function, with bounded derivatives on  $[0, T]$ .*

1. *With probability 1, for any  $t \in [0, T]$  we have*

$$\int_0^t f(s) dW_s = f(t)W_t - \int_0^t W_s f'(s) ds. \quad (3.6)$$

2. *The process  $\{\int_0^t f(s) dW_s ; t \in [0, T]\}$  is a continuous Gaussian process, with zero mean and with a covariance function*

$$\mathbb{Cov}\left(\int_0^t f(u) dW_u, \int_0^s f(u) dW_u\right) = \int_0^{s \wedge t} f^2(u) du. \quad (3.7)$$

3. *For another function  $g$  satisfying the same assumptions, we have*

$$\mathbb{Cov}\left(\int_0^t f(u) dW_u, \int_0^s g(u) dW_u\right) = \int_0^{s \wedge t} f(u)g(u) du. \quad (3.8)$$

PROOF :

The first item is a direct application of Theorem 3.6 to the function  $(t, x) \mapsto f(t)x$ .

For any coefficients  $(\alpha_i)_{1 \leq i \leq N}$  and times  $(T_i)_{1 \leq i \leq N}$ ,  $\sum_{i=1}^N \alpha_i \int_0^{T_i} f(u) dW_u$  is a Gaussian r.v. since it can be written as a limit of Gaussian r.v. of the form  $\sum_j \beta_j (W_{t_{j+1}} - W_{t_j})$ : thus,  $\{\int_0^t f(s) dW_s ; t \in [0, T]\}$  is a Gaussian process. Its continuity is obvious in view of (3.6). Its expectation is the limit of the expectation of  $\sum_{t_i \leq t} f(t_i) [W_{t_{i+1}} - W_{t_i}]$ , thus equal to 0. The covariance is the limit of the covariance

$$\begin{aligned} & \mathbb{Cov}\left(\sum_{t_i \leq t} f(t_i) [W_{t_{i+1}} - W_{t_i}], \sum_{t_j \leq s} f(t_j) [W_{t_{j+1}} - W_{t_j}]\right) \\ &= \sum_{t_i \leq t, t_j \leq s} f(t_i) f(t_j) \mathbb{Cov}(W_{t_{i+1}} - W_{t_i}, W_{t_{j+1}} - W_{t_j}) \\ &= \sum_{t_i \leq t, t_j \leq s} f(t_i) f(t_j) \delta_{i,j} (t_{i+1} - t_i) \xrightarrow{n \rightarrow +\infty} \int_0^{s \wedge t} f^2(u) du. \end{aligned}$$

The second item is proved. The last item is proved similarly.  $\square$

As a consequence, going back to the Ornstein-Uhlenbeck process (Paragraph 1.6.2), we can complete the proof of its representation (1.11) using a stochastic integral, starting from (1.10). For this apply the result below to the function  $f(s) = e^{-a(t-s)}$  ( $t$  fixed): it gives  $\int_0^t e^{-a(t-s)} dW_s = W_t - a \int_0^t e^{-a(t-s)} W_s ds$ . It leads to

$$V_t = v_0 e^{-at} + \sigma \int_0^t e^{-a(t-s)} dW_s. \quad (3.9)$$

Then the Gaussian property from Proposition 3.8 gives that the variance of  $V_t$  is equal to  $\sigma^2 \int_0^t e^{-2a(t-s)} ds = \frac{\sigma^2}{2a} (1 - e^{-2at})$ .

### 3.4 Itô formula for other processes

The reader should have noticed that the central property for the proof of Theorem 3.6 is that the BM has a finite quadratic variation. Thus, the Itô formula can directly be extended to processes  $X$  which enjoy the same property.

#### 3.4.1 The one-dimensional case

In this paragraph, we first consider scalar processes. The multidimensional extension is made afterwards.

**Definition 3.9 (Quadratic variation of a process)** *A continuous process  $X$  has a finite quadratic variation if for any  $t \geq 0$ , the limit*

$$V_t^n = \sum_{t_i \leq t} (X_{t_{i+1}} - X_{t_i})^2 \quad (3.10)$$

*along the dyadic subdivision of order  $n$ , exists a.s. and is finite. We denote this limit by  $\langle X \rangle_t$  et it is usually called the bracket of  $X$  at time  $t$ .*

If  $X = W$  is a BM, we have  $\langle X \rangle_t = t$ . More generally, it is easy to check that  $\langle X \rangle$  is increasing and continuous. We associate to it a positive measure and this extends Proposition 3.5 to  $X$ .

**Proposition 3.10** *For any continuous function  $f$ , with probability 1 for any  $t \geq 0$  we have*

$$\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f(t_i) (X_{t_{i+1}} - X_{t_i})^2 = \int_0^t f(s) d\langle X \rangle_s.$$

Theorem 3.6 becomes

**Theorem 3.11 (Itô formula for  $X$ )** *Let  $f \in \mathcal{C}^{1,2}(\mathbb{R}^+ \times \mathbb{R}, \mathbb{R})$  and  $X$  be with finite quadratic variation. With probability 1, for any  $t \geq 0$  we have*

$$f(t, X_t) = f(0, X_0) + \int_0^t f'_x(s, X_s) dX_s + \int_0^t f'_t(s, X_s) ds + \frac{1}{2} \int_0^t f''_{xx}(s, X_s) d\langle X \rangle_s, \quad (3.11)$$

*where  $\int_0^t f'_x(s, X_s) dX_s$  is the stochastic integral of  $f'_x(s, X_s)$  w.r.t.  $X$  and it is the a.s. limit of  $\sum_{t_i \leq t} f'_x(t_i, X_{t_i}) (X_{t_{i+1}} - X_{t_i})$  along dyadic subdivision of order  $n$ .*

Often, the Itô formula is written formally under a differential form

$$df(t, X_t) = f'_x(t, X_t) dX_t + f'_t(t, X_t) dt + \frac{1}{2} f''_{xx}(t, X_t) d\langle X \rangle_t.$$

We now provide hand-made tools to compute the bracket of  $X$  in practice.

**Proposition 3.12 (Computation of the bracket)** *Let  $A$  and  $M$  two continuous processes such that  $A$  has a finite variation <sup>17</sup> and  $M$  has a finite quadratic variation:*

1.  $\langle A \rangle_t = 0$ ;
2. if  $X_t = x + M_t$ , then  $\langle X \rangle_t = \langle M \rangle_t$ ;
3. if  $X_t = \lambda M_t$ , then  $\langle X \rangle_t = \lambda^2 \langle M \rangle_t$ ;
4. if  $X_t = M_t + A_t$ , then  $\langle X \rangle_t = \langle M \rangle_t$ ;
5. if  $X_t = f(A_t, M_t)$  with  $f \in C^1$ , then  $\langle X \rangle_t = \int_0^t [f'_m(A_s, M_s)]^2 d\langle M \rangle_s$ .

The proof is easy and it uses deterministic arguments based on the definition of  $\langle X \rangle$ , we skip it. Item 5) shows that the class of processes with finite quadratic variation is stable by smooth composition. The following examples are important.

### Examples 3.13

- **Arithmetic Brownian Motion** ( $X_t = x + bt + \sigma W_t$ ): we have

$$\langle X \rangle_t = \langle \sigma W \rangle_t = \sigma^2 \langle W \rangle_t = \sigma^2 t.$$

Itô's formula becomes

$$\begin{aligned} df(t, X_t) &= (f'_t(t, X_t) + f'_x(t, X_t)b + \frac{1}{2} f''_{xx}(t, X_t)\sigma^2)dt + f'_x(t, X_t)\sigma dW_t \\ &:= (f'_t(t, X_t) + L_{b, \sigma^2}^{\text{ABM}} f(t, X_t))dt + f'_x(t, X_t)\sigma dW_t. \end{aligned} \quad (3.12)$$

An important example is associated to  $f(x) = \exp(x)$ :

$$d[\exp(X_t)] = \exp(X_t)(b + \frac{1}{2}\sigma^2)dt + \exp(X_t)\sigma dW_t. \quad (3.13)$$

- **Geometric Brownian Motion** ( $S_t = S_0 e^{(\mu - \frac{1}{2}\sigma^2)t + \sigma W_t}$ ): we have

$$\langle S \rangle_t = \int_0^t \sigma^2 S_s^2 ds.$$

From (3.13), we obtain a linear equation for the dynamics of  $S$ :

$$dS_t = S_t \mu dt + S_t \sigma dW_t$$

also written  $\frac{dS_t}{S_t} = \mu dt + \sigma dW_t$  putting an emphasize of the financial interpretation as returns. The Itô formula writes

$$\begin{aligned} df(t, S_t) &= (f'_t(t, S_t) + f'_x(t, S_t)S_t\mu + \frac{1}{2} f''_{xx}(t, S_t)S_t^2\sigma^2)dt + f'_x(t, S_t)\sigma S_t dW_t \\ &:= (f'_t(t, S_t) + L_{\mu, \sigma^2}^{\text{GBM}} f(t, S_t))dt + f'_x(t, S_t)\sigma S_t dW_t. \end{aligned} \quad (3.14)$$

---

<sup>17</sup>i.e. the sum of  $\sum_{t_i \leq t} |A_{t_{i+1}} - A_{t_i}|$  exists and is finite, for instance  $A \in C^1$ .

- **Ornstein-Uhlenbeck process** ( $V_t = v_0 - a \int_0^t V_s ds + \sigma W_t$ ): we have

$$\langle V \rangle_t = \sigma^2 t.$$

The Itô formula follows

$$\begin{aligned} df(t, V_t) &= (f'_t(t, V_t) - a f'_x(t, V_t) V_t + \frac{1}{2} \sigma^2 f''_{xx}(t, V_t)) dt + f'_x(t, V_t) \sigma dW_t \\ &:= (f'_t(t, V_t) + L_{a, \sigma^2}^{\text{OU}} f(t, V_t)) dt + f'_x(t, V_t) \sigma dW_t. \end{aligned} \quad (3.15)$$

- **Euler scheme defined in (1.12)** ( $X_t^h = X_{ih}^h + b(X_{ih}^h)(t - ih) + \sigma(X_{ih}^h)(W_t - W_{ih})$  for  $i \geq 0, t \in (ih, (i+1)h]$ ). Since  $X^h$  is an arithmetic BM on each interval  $(ih, (i+1)h]$ , we easily obtain

$$\langle X^h \rangle_t = \int_0^t \sigma^2(\varphi(s), X_{\varphi(s)}^h) ds$$

where  $\varphi(t) = ih$  for  $t \in (ih, (i+1)h]$ . The Itô formula writes

$$\begin{aligned} df(t, X_t^h) &= (f'_t(t, X_t^h) + b(X_{\varphi(t)}^h) f'_x(t, X_t^h) + \frac{1}{2} \sigma^2(X_{\varphi(t)}^h) f''_{xx}(t, X_t^h)) dt \\ &\quad + f'_x(t, X_t^h) \sigma(X_{\varphi(t)}^h) dW_t. \end{aligned} \quad (3.16)$$

### 3.4.2 The multidimensional case

We briefly expose the situation when  $X = (X_1, \dots, X_d)$  takes values in  $\mathbb{R}^d$ . The main novelty consists in considering the cross quadratic variation defined by the limit (assuming its existence, along dyadic subdivision) of

$$\langle X_k, X_l \rangle_t^n = \sum_{t_i \leq t} (X_{k, t_{i+1}} - X_{k, t_i})(X_{l, t_{i+1}} - X_{l, t_i}) \xrightarrow{n \rightarrow +\infty} \langle X_k, X_l \rangle_t. \quad (3.17)$$

We list basic properties.

#### Properties 3.14

1. SYMMETRY:  $\langle X_k, X_l \rangle_t = \langle X_l, X_k \rangle_t$ .
2. USUAL BRACKET:  $\langle X_k, X_k \rangle_t = \langle X_k \rangle_t$ .
3. POLARIZATION:  $\langle X_k, X_l \rangle_t = \frac{1}{4} (\langle X_k + X_l \rangle_t - \langle X_k - X_l \rangle_t)$ .
4.  $\langle \cdot, \cdot \rangle_t$  is bilinear.
5. For any continuous function  $f$ , we have

$$\lim_{n \rightarrow \infty} \sum_{t_i \leq t} f(t_i) (X_{k, t_{i+1}} - X_{k, t_i})(X_{l, t_{i+1}} - X_{l, t_i}) = \int_0^t f(s) d\langle X_k, X_l \rangle_s.$$

6. Let  $X_{1,t} = f(A_{1,t}, M_{1,t})$  and  $X_{2,t} = g(A_{2,t}, M_{2,t})$ , where the variation (resp. quadratic variation) of  $A = (A_1, A_2)$  (resp.  $M = (M_1, M_2)$ ) is finite, and let  $f$  and  $g$  be two  $\mathcal{C}^1$ -functions: we have

$$\langle X_1, X_2 \rangle_t = \int_0^t f'_m(A_{1,s}, M_{1,s}) g'_m(A_{2,s}, M_{2,s}) d\langle M_1, M_2 \rangle_s.$$

In particular,  $\langle A_1 + M_1, A_2 + M_2 \rangle_t = \langle M_1, M_2 \rangle_t$ .

7. Let  $W_1$  and  $W_2$  be two independent Brownian motions: then

$$\langle W_1, W_2 \rangle_t = 0.$$

PROOF :

The statements 1)-6) are easy to check from the definition or using previous arguments. The statement 7) is important and we give details: use the polarization identity

$$\langle W_1, W_2 \rangle_t = \frac{1}{4} (\langle W_1 + W_2 \rangle_t - \langle W_1 - W_2 \rangle_t).$$

We observe that both  $\frac{1}{\sqrt{2}}(W_1 + W_2)$  and  $\frac{1}{\sqrt{2}}(W_1 - W_2)$  are Brownian motions, since each one is a continuous Gaussian process with the right covariance function. Thus,  $\langle \frac{1}{\sqrt{2}}(W_1 + W_2) \rangle_t = \langle \frac{1}{\sqrt{2}}(W_1 - W_2) \rangle_t = t$  and the result follows.  $\square$

The Itô formula naturally extends to this setting.

**Theorem 3.15 (Multidimensional Itô formula)** *Let  $f \in \mathcal{C}^{1,2}(\mathbb{R}^+ \times \mathbb{R}^d, \mathbb{R})$  and  $X$  be a continuous  $d$ -dimensional process with finite quadratic variation. Then, with probability 1, for any  $t \geq 0$  we have*

$$\begin{aligned} f(t, X_t) &= f(0, X_0) + \sum_{k=1}^d \int_0^t f'_{x_k}(s, X_s) dX_{k,s} + \int_0^t f'_t(s, X_s) ds \\ &\quad + \frac{1}{2} \sum_{k,l=1}^d \int_0^t f''_{x_k, x_l}(s, X_s) d\langle X_k, X_l \rangle_s \end{aligned}$$

where the sum of stochastic integrals are defined as before.

In particular, the integration by parts formula writes

$$X_{1,t} X_{2,t} = X_{1,0} X_{2,0} + \int_0^t X_{1,s} dX_{2,s} + \int_0^t X_{2,s} dX_{1,s} + \langle X_1, X_2 \rangle_t.$$

For two independent Brownian motions, we recover the usual deterministic formula (because  $\langle W_1, W_2 \rangle_t = 0$ ), but in general, formulas are different because of the quadratic variation.



### 3.5 More properties on stochastic integrals

So far, we have defined some specific stochastic integrals, those appearing in deriving a Itô formula and which have the form

$$\int_0^t f'_x(s, X_s) dX_s = \lim_{n \rightarrow +\infty} \sum_{t_i \leq t} f'_x(t_i, X_{t_i})(X_{t_{i+1}} - X_{t_i}), \quad (3.18)$$

the limit being taken along dyadic subdivision. Also, we have proved that if  $f$  has bounded derivatives and  $X = W$  is a Brownian motion, the above stochastic integral must have zero-expectation (see equality (3.4)). Moreover, we also have established that in the case of deterministic integrand (Wiener integral), the second moment of the stochastic integral is explicit and given by

$$\mathbb{E}(\int_0^t h_s dW_s)^2 = \int_0^t h_s^2 ds.$$

The aim of this paragraph is to provide extension of the above properties on the two first moments to more general integrands, under some suitable boundedness or integrability conditions.

#### 3.5.1 Heuristic arguments

In view of the previous construction, there is a natural candidate to be the stochastic integral  $\int_0^t h_s dW_s$ . When  $h$  is piecewise constant process (called *simple process*), that is  $h_s = h_{t_i}$  if  $s \in [t_i, t_{i+1}]$  for a given deterministic time grid  $(t_i)_i$ , we set

$$\int_0^t h_s dW_s = \sum_{t_i \leq t} h_{t_i}(W_{t \wedge t_{i+1}} - W_{t_i}), \quad (3.19)$$

Without extra assumptions on the stochasticity of  $h$ , it is not clear why its expectation equals 0. This property should come from the centered Brownian increments  $W_{t \wedge t_{i+1}} - W_{t_i}$  and their independence to  $h_{t_i}$  so that

$$\mathbb{E}(\int_0^t h_s dW_s) = \sum_{t_i \leq t} \mathbb{E}(h_{t_i}) \mathbb{E}(W_{t \wedge t_{i+1}} - W_{t_i}) = 0.$$

To validate this computation, we shall assume that  $h_t$  depends only the Brownian Motion  $W$  before  $t$  and it is integrable. To go to the second moment, assume additionally that  $h$  is square integrable: then

$$\begin{aligned} & \mathbb{E}|\int_0^t h_s dW_s|^2 \\ &= 2 \sum_{t_i < t_j \leq t} \mathbb{E}(h_{t_i} h_{t_j} (W_{t \wedge t_{i+1}} - W_{t_i})) \mathbb{E}(W_{t \wedge t_{j+1}} - W_{t_j}) + \sum_{t_i \leq t} \mathbb{E}(h_{t_i}^2) \mathbb{E}|W_{t \wedge t_{i+1}} - W_{t_i}|^2 \\ &= \sum_{t_i \leq t} \mathbb{E}(h_{t_i}^2) (t \wedge t_{i+1} - t_i) = \mathbb{E}(\int_0^t h_s^2 ds). \end{aligned} \quad (3.20)$$

This equality should be read as an isometry property (usually referred to as *Itô isometry*), on which we can rely an extension of the stochastic integral of simple process to more general process. At this point, we should need to enter into measurability considerations to describe what " *$h_t$  depends only the Brownian Motion  $W$  before  $t$* " means at the most general level. It goes far beyond this introductory lecture: for the exposure of the general theory, see for instance [KS91] or [RY05].

For most of the examples considered in these lectures, we can restrict to *very good integrands*, in the sense that a integrand  $h$  is *very good* if

1.  $(h_t)_t$  is continuous or piecewise continuous (as for simple processes);
2. for a given  $t$ ,  $h_t$  is a continuous functional of  $(W_s : s \leq t)$ ;
3. it is square integrable in time and  $\omega$ :  $\mathbb{E}(\int_0^t h_s^2 ds) < +\infty$  for any  $t$ .

This setting ensures that we can define stochastic integrals for very good integrands as the  $L_2$ -limit of stochastic integrals for simple integrands: indeed, a Cauchy sequence  $(h_n)_n$  in  $L_2(dt \otimes d\mathbb{P})$  gives a Cauchy sequence  $(\int_0^t h_{n,s} dW_s)_n$  in  $L_2(\mathbb{P})$  due to the isometry (3.20).

### 3.5.2 General results

We collect here all the stochastic integration results needed in these lectures.

**Theorem 3.16** *Let  $h$  be a very good integrand. Then the stochastic integral  $\int_0^t h_s dW_s$  is such that*

1. *it is the  $L_2$  limit of  $\sum_{t_i \leq t} h_{t_i}(W_{t \wedge t_{i+1}} - W_{t_i})$  along time subdivision which time step goes to 0;*
2. *it is centered:  $\mathbb{E}(\int_0^t h_s dW_s) = 0$ ;*
3. *it is square integrable:  $\mathbb{E}|\int_0^t h_s dW_s|^2 = \mathbb{E}(\int_0^t h_s^2 ds)$ ,*
4. *for two very good integrands  $h_1$  and  $h_2$ , we have*

$$\mathbb{E}\left[\left(\int_0^t h_{1,s} dW_s\right)\left(\int_0^t h_{2,s} dW_s\right)\right] = \mathbb{E}\left(\int_0^t h_{1,s} h_{2,s} ds\right).$$

Beyond the  $t$ -by- $t$  construction, actually the full theory gives a construction for any  $t$  simultaneously, proving additionally time continuity property, general centering property (*martingale* property), tight  $L_p$ -estimates on the value at time  $t$  and the extrema until time  $t$  (Burkholder-Davis-Gundy inequalities) and so one... For multidimensional  $W$  and  $h$ , the construction should be understood component wise. Another fruitful extension is to allow  $t$  to be a bounded stopping time, similarly to the discussion we have made in the proof of Theorem 2.4.

Another interesting part in the theory is devoted to the existence and uniqueness of solution to Stochastic Differential Equations (also known as diffusion processes). The easiest setting is to assume globally Lipschitz coefficients: it is similar to the ODE framework, and the proof is also based on the Picard fixed-point argument. We state the results without proof.

**Theorem 3.17** *Let  $W$  be a  $d$ -dimensional standard Brownian motion.*

*Assume that the functions  $b : \mathbb{R}^d \mapsto \mathbb{R}^d$  and  $\sigma : \mathbb{R}^d \mapsto \mathbb{R}^d \otimes \mathbb{R}^d$  are globally Lipschitz. Then, for any initial condition  $x \in \mathbb{R}^d$ , there exists a unique<sup>18</sup> continuous solution  $(X_t^x)_{t \geq 0}$  valued in  $\mathbb{R}^d$  which satisfies*

$$X_t^x = x + \int_0^t b(X_s^x) ds + \int_0^t \sigma(X_s^x) dW_s, \quad (3.21)$$

*with  $\sup_{0 \leq t \leq T} \mathbb{E}|X_t^x|^2 < +\infty$  for any given  $T \in \mathbb{R}^+$ .*

*The continuous process  $X^x$  has a finite quadratic variation given by*

$$\langle X_k^x, X_l^x \rangle_t = \int_0^t [\sigma \sigma^\perp]_{k,l}(X_s^x) ds, \quad 1 \leq k, l \leq d. \quad (3.22)$$

Observe that this general result includes all the model considered before, such as Arithmetic and Geometric Brownian Motion, Ornstein-Uhlenbeck processes, here stated in a possibly multidimensional framework.

**Complementary references:** see [KS91] and [RY05].

## 4 Monte Carlo resolutions of linear PDEs related to SDEs

The use of probabilistic methods to solve PDEs have become very popular during the two last decades. They are usually not competitive compared to deterministic methods in low dimension, but for higher dimension they provide very good alternative schemes. In the sequel, we give a brief introduction to the topics, relying on the material presented in the previous sections. We start with linear parabolic PDEs, with Cauchy-Dirichlet boundary conditions. Next section is devoted to semi-linear PDEs.

### 4.1 Second order linear parabolic PDEs with Cauchy initial condition

#### 4.1.1 Feynman-Kac formulas

We start with a verification Theorem generalizing Theorems 2.1, 2.6, 2.9 to the case of general SDEs. We incorporate a source term  $g$ .

**Theorem 4.1** *Under the assumptions of Theorem 3.17, let  $X^x$  be the solution (3.21) starting from  $x \in \mathbb{R}^d$  and set*

$$L_{b, \sigma \sigma^\perp}^X = \frac{1}{2} \sum_{i,j=1}^d [\sigma \sigma^\perp]_{i,j}(x) \partial_{x_i x_j}^2 + \sum_{i=1}^d b_i(x) \partial_{x_i}.$$

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<sup>18</sup>up to a set of zero probability measure

Assume there is a solution  $u \in \mathcal{C}_b^{1,2}(\mathbb{R}^+ \times \mathbb{R}^d, \mathbb{R})$  to the PDE

$$\begin{cases} u'_t(t, x) = L_{b, \sigma \sigma^\perp}^X u(t, x) + g(x), \\ u(0, x) = f(x). \end{cases} \quad (4.1)$$

for two given functions  $f, g : \mathbb{R}^d \rightarrow \mathbb{R}$ . Then  $u$  is given by

$$u(t, x) = \mathbb{E}[f(X_t^x) + \int_0^t g(X_s^x) ds]. \quad (4.2)$$

PROOF :

Let  $t$  be fixed. We apply the general Itô formula (Theorem 3.15) to the process  $X^x$  and to the function  $v : (s, y) \mapsto u(t - s, y)$ : it gives

$$dv(s, X_s^x) = [v'_s(s, X_s^x) + L_{b, \sigma \sigma^\perp}^X v(s, X_s^x)] ds + Dv(s, X_s^x) \sigma(X_s^x) dW_s \quad (4.3)$$

$$= -g(X_s^x) ds + Dv(s, X_s^x) \sigma(X_s^x) dW_s. \quad (4.4)$$

Observe that the integrand  $h_s = Dv(s, X_s^x) \sigma(X_s^x)$  is very good, since  $v$  has bounded derivatives,  $\sigma$  has a linear growth, and  $X_s$  has bounded second moments, locally uniformly in  $s$ : thus, the stochastic integral  $\int_0^t Dv(s, X_s^x) \sigma(X_s^x) dW_s$  has zero expectation. Hence, applying the above decomposition between  $s = 0$  and  $s = t$  and taking the expectation, it gives

$$\mathbb{E}(f(X_t^x)) = \mathbb{E}(v(t, X_t^x)) = v(0, x) - \mathbb{E}\left(\int_0^t g(X_s^x) ds\right) = u(t, x) - \mathbb{E}\left(\int_0^t g(X_s^x) ds\right).$$

We are done.  $\square$

Smoothness assumptions on  $u$  are satisfied in  $f, g$  are smooth enough. If not, and a uniform ellipticity condition is met on  $\sigma \sigma^\perp$ , the fundamental solution of the PDE is smoothing the data and the result can be extended. However, the derivatives blow up as time goes to 0, and more technicalities are necessary to justify the same stochastic calculus computations. The fundamental solution  $p(t, x, y)$  has a simple probabilistic interpretation: it is the density of  $X_t^x$  at  $y$ . Indeed, identify  $\mathbb{E}[f(X_t^x) + \int_0^t g(X_s^x) ds]$  with

$$u(t, x) = \int_{\mathbb{R}^d} p(t, x, y) f(y) dy + \int_0^t \int_{\mathbb{R}^d} p(s, x, y) g(y) dy ds.$$

#### 4.1.2 Monte Carlo schemes

Since  $u(t, x)$  is represented as an expectation, it allows the use of a Monte Carlo method to numerically compute the solution. The difficulty is that in general,  $X$  can not simulated perfectly accurately, only an approximation on a finite time-grid can be simply and efficiently produced. Namely we use the Euler scheme with time step  $h = t/N$ :

$$\begin{cases} X_0^{x,h} = x, \\ X_s^{x,h} = X_{ih}^{x,h} + b(X_{ih}^{x,h})(s - ih) + \sigma(X_{ih}^{x,h})(W_s - W_{ih}), \quad i \geq 0, \quad s \in (ih, (i+1)h]. \end{cases} \quad (4.5)$$

Observe that to get  $X_t^{x,h}$ , we do not need to sample the continuous path of  $X^{x,h}$  (as difficult as having a continuous path of a BM): in fact, we only need to compute  $X_{ih}^{x,h}$  iteratively for  $i = 0$  to  $i = N$ . Each time iteration requires to sample  $d$  new independent Gaussian increments  $W_{k,(i+1)h} - W_{k,ih}$ , centered with variance  $h$ : it is straightforward. The computational cost is essentially equal to  $C(d)N$  where the constant depends on the dimension (coming from  $d$ -dimensional vector and matrix computations).

As an approximation of the expectation of  $\mathcal{E}(f, g, X^x) = f(X_t^x) + \int_0^t g(X_s^x)ds$ , we take the expectation

$$\mathcal{E}(f, g, X^{x,h}) = f(X_{Nh}^{x,h}) + \sum_{i=0}^{N-1} g(X_{ih}^{x,h})h, \quad (4.6)$$

a random variable of which we sample  $M$  independent copies, that are denoted by  $\{\mathcal{E}(f, g, X^{x,h,m}) : 1 \leq m \leq M\}$ . Then, the Monte Carlo approximation, based on this sample of  $M$  Euler schemes with time step  $h$ , is

$$\begin{aligned} \frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) &= u(t, x) + \underbrace{\frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) - \mathbb{E}(\mathcal{E}(f, g, X^{x,h}))}_{\text{statistical error Err.stat.}(h,M)} \\ &\quad + \underbrace{\mathbb{E}(\mathcal{E}(f, g, X^{x,h})) - u(t, x)}_{\text{discretization error Err.disc.}(h)}. \end{aligned} \quad (4.7)$$

The first error contribution is due to the sample of finite size: the larger  $M$ , the better the accuracy. As mentioned in Paragraph 2.1.3, once renormalized by  $\sqrt{M}$ , this error is still random and its distribution is closed to the Gaussian distribution with zero mean and variance  $\text{Var}(\mathcal{E}(f, g, X^{x,h}))$ : the latter still depends on  $h$  but very little, since it is expected to be close to  $\text{Var}(\mathcal{E}(f, g, X^x))$ .

The second error contribution is related to the time discretization effect: the smaller the time  $h$ , the better the accuracy. In the sequel (Paragraph 4.1.3), we theoretically estimate this error in terms of  $h$ , and proves that it is of order  $h$  (even equivalent to) under some reasonable and fairly general assumptions.

**What is the optimal tuning of  $h \rightarrow 0$  and  $M \rightarrow +\infty$ ?** An easy complexity analysis shows that the computational effort is  $\mathcal{C}_e = C(d)Mh^{-1}$ . Observe that it does not depend on the dimension  $d$ , as a difference with a PDE method, but on the other hand, the solution is computed only at single point  $(t, x)$ . The squared quadratic error is equal to

$$\begin{aligned} [\text{Err}_2(h, M)]^2 &:= \mathbb{E} \left[ \frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) - u(t, x) \right]^2 \\ &= \frac{\text{Var}(\mathcal{E}(f, g, X^{x,h}))}{M} + \left[ \mathbb{E}(\mathcal{E}(f, g, X^{x,h})) - u(t, x) \right]^2. \end{aligned}$$

Only the first factor  $\text{Var}(\mathcal{E}(f, g, X^{x,h}))$  can be estimated with the same sample, for  $M$  large, and it depends little of  $h$ . Say that the second term is equivalent to  $(Ch)^2$  as  $h \rightarrow 0$ , with  $C \neq 0$ . Then, three asymptotic situations occur:

1. If  $M \gg h^{-2}$ , the statistical error becomes negligible and  $\frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) - u(t, x) \sim Ch$ . The computational effort is  $\mathcal{C}_e \gg h^{-3}$  and thus  $\text{Err}_2(h, M) \gg \mathcal{C}_e^{-1/3}$ . Deriving a confidence interval as in Paragraph 2.1.3 is meaningless, we face with the discretization error only.
2. If  $M \ll h^{-2}$ , the discretization error becomes negligible and the distribution of  $\sqrt{M} \left( \frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) - u(t, x) \right)$  converges to that a Gaussian r.v. centered with variance  $\text{Var}(\mathcal{E}(f, g, X^x))$  (that can be asymptotically computed using the  $M$ - sample). Thus, we can derive confidence intervals: setting  $\sigma_{h,M}^2$  the empirical variance of  $\mathcal{E}(f, g, X^{x,h})$ , with probability 95% we have

$$u(t, x) \in \left[ \frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) - 1.96 \frac{\sigma_{h,M}}{\sqrt{M}}, \frac{1}{M} \sum_{m=1}^M \mathcal{E}(f, g, X^{x,h,m}) + 1.96 \frac{\sigma_{h,M}}{\sqrt{M}} \right].$$

Regarding the computational effort, we have  $\mathcal{C}_e \gg M^{3/2}$  and thus  $\text{Err}_2(h, M) \gg \mathcal{C}_e^{-1/3}$ .

3. If  $M \sim ch^{-2}$ , both statistical and discretization errors have the same magnitude and one can still derive a asymptotic confidence interval, but it is no more centered (as in  $M \ll h^{-2}$ ) and unfortunately, the bias is not easily estimated on the fly. The problem is that the bias is of same magnitude as the size of the confidence interval, thus it reduces the interest of having such a priori statistical error estimate. Here,  $\text{Err}_2(h, M) = O(\mathcal{C}_e^{-1/3})$ .

Summing up by considering the ability of having or not on-line error estimates and by optimizing the final accuracy w.r.t. the computational effort, the second case  $M = h^{-2+\varepsilon}$  (for a small  $\varepsilon > 0$ ) may be the most attractive since it achieves (almost) the best accuracy w.r.t. the computational effort and gives a centered confidence interval (and therefore tractable and meaningful error bounds).

#### 4.1.3 Convergence of the Euler scheme

An important issue is to analyze the impact of time discretization of SDE. This dates back to the end of eighties, see [TL90] among others. The result below gives a mathematical justification of the use of the Euler scheme as an approximation for the distribution of the SDE.

**Theorem 4.2** *Assume that  $b$  and  $\sigma$  are  $\mathcal{C}_b^2$ , let  $X^x$  be the solution (3.21) starting from  $x \in \mathbb{R}^d$  and let  $X^{h,x}$  be its Euler scheme defined in (4.5). Assume that  $u(t, x) = \mathbb{E}[f(X_t^x) + \int_0^t g(X_s^x) ds]$  is a  $\mathcal{C}_b^{2,4}([0, T] \times \mathbb{R}^d, \mathbb{R})$ -function solution of the PDE of Theorem 4.1. Then,*

$$\mathbb{E} \left[ f(X_{Nh}^{x,h}) + \sum_{i=0}^{N-1} g(X_{ih}^{x,h}) h \right] - \mathbb{E} \left[ f(X_t^x) + \int_0^t g(X_s^x) ds \right] = O(h).$$

PROOF :

Denote by  $\text{Err}_{\text{disc.}}(h)$  the above discretization error. As in Theorem 4.1, we use the

function  $v : (s, y) \mapsto u(t - s, y)$  (for a fixed  $t$ ) and we apply the Itô formula to  $X^{h,x}$  (Theorem 3.15): it gives

$$\begin{aligned}
dv(s, X_s^{h,x}) &= \left[ v'_s(s, X_s^{h,x}) + \frac{1}{2} \sum_{i,j=1}^d [\sigma \sigma^\perp]_{i,j}(X_{\varphi(s)}^{h,x}) \partial_{x_i x_j}^2 v(s, X_s^{h,x}) \right. \\
&\quad \left. + \sum_{i=1}^d b_i(X_{\varphi(s)}^{h,x}) \partial_{x_i} v(s, X_s^{h,x}) \right] ds + Dv(s, X_s^{h,x}) \sigma(X_{\varphi(s)}^{h,x}) dW_s. \\
&= \left[ \frac{1}{2} \sum_{i,j=1}^d ([\sigma \sigma^\perp]_{i,j}(X_{\varphi(s)}^{h,x}) - [\sigma \sigma^\perp]_{i,j}(X_s^{h,x})) \partial_{x_i x_j}^2 v(s, X_s^{h,x}) \right. \\
&\quad \left. + \sum_{i=1}^d (b_i(X_{\varphi(s)}^{h,x}) - b_i(X_s^{h,x})) \partial_{x_i} v(s, X_s^{h,x}) - g(X_s^{h,x}) \right] ds \\
&\quad + Dv(s, X_s^{h,x}) \sigma(X_{\varphi(s)}^{h,x}) dW_s.
\end{aligned}$$

where at the second equality, we have used the PDE solved by  $v$  at  $(s, X_s^x)$ . Then, by taking the expectation (it removes the stochastic integral term because the integrand is very good), we obtain

$$\begin{aligned}
\text{Err}_{\text{disc.}}(h) &= \mathbb{E} \left[ v(Nh, X_{Nh}^{x,h}) + \sum_{i=1}^N hg(X_{ih}^{x,h}) \right] - v(0, x) \\
&= \mathbb{E} \left( \int_0^t \left[ \frac{1}{2} \sum_{i,j=1}^d ([\sigma \sigma^\perp]_{i,j}(X_{\varphi(s)}^{h,x}) - [\sigma \sigma^\perp]_{i,j}(X_s^{h,x})) \partial_{x_i x_j}^2 v(s, X_s^{h,x}) \right] ds \right) \\
&\quad + \mathbb{E} \left( \int_0^t \left[ \sum_{i=1}^d (b_i(X_{\varphi(s)}^{h,x}) - b_i(X_s^{h,x})) \partial_{x_i} v(s, X_s^{h,x}) \right] ds \right) \\
&\quad + \mathbb{E} \left( \int_0^t [g(X_{\varphi(s)}^{h,x}) - g(X_s^{h,x})] ds \right).
\end{aligned}$$

The global error is represented as a summation of local errors. For instance, let us estimate the first term related to  $\sigma \sigma^\perp$ : apply once again the Itô formula on the interval  $[kh, s] \subset [kh, (k+1)h]$  and to the function  $(s, y) \mapsto ([\sigma \sigma^\perp]_{i,j}(X_{\varphi(s)}^{h,x}) - [\sigma \sigma^\perp]_{i,j}(y)) \partial_{x_i x_j}^2 v(s, y)$ . It gives raise to a time integral between  $kh = \varphi(s)$  and  $s$  and a stochastic integral that vanishes in expectation. Proceed similarly for the other contributions with  $b$  and  $g$ . Finally we obtain a representation formula of the form

$$\text{Err}_{\text{disc.}}(h) = \sum_{\alpha: 0 \leq |\alpha| \leq 4} \mathbb{E} \left( \int_0^t \int_{\varphi(s)}^s \partial_x^{|\alpha|} v(r, X_r^{h,x}) l_\alpha(X_{\varphi(r)}^{h,x}, X_r^{h,x}) dr ds \right)$$

where the summation is made on differentiation multi-indices of length smaller than 4, where  $l_\alpha$  are functions depending on  $b, \sigma, g$  and their derivatives up to order 2, and where  $l_\alpha$  has at most a linear growth w.r.t its two variables. Taking advantage of the boundedness of the derivatives of  $v$ , we easily complete the proof.

Observe that, by strengthening the assumptions and by going a bit further in the analysis, we could establish an expansion w.r.t.  $h$ .  $\square$

The previous assumption on  $u$  implies that  $f \in \mathcal{C}_b^4$  and  $g \in \mathcal{C}_b^2$ , which is too strong in practice. The extension to non smooth  $f$  is much more difficult and we have to take advantage of the smoothness coming from the non-degenerate distribution of  $X$  or  $X^h$ . We may follow the same types of computations, mixing PDE techniques and stochastic arguments, see [BT96]. But this is a pure stochastic analysis approach (Malliavin calculus) which provides the extension under the minimal non-degeneracy assumption (i.e. only stated at the initial point  $x$ ), see [GM05c]. We state the result without proofs.

**Theorem 4.3** *Assume that  $b$  and  $\sigma$  are  $\mathcal{C}_b^\infty$ , let  $X^x$  be the solution (3.21) starting from  $x \in \mathbb{R}^d$  and let  $X^{h,x}$  be its Euler scheme defined in (4.5). Assume additionally that  $\sigma\sigma^\perp(x)$  is invertible. Then, for any bounded measurable function  $f$ , we have*

$$\mathbb{E}\left[f(X_t^{x,h})\right] - \mathbb{E}\left[f(X_t^x)\right] = O(h).$$

In the same reference [GM05c], the result is also proved for hypoelliptic system, where the hypoellipticity holds only at the starting point  $x$ . On the other hand, without such a degeneracy condition and for non smooth  $h$  (like Heaviside function), the convergence may fail.

The case of coefficients  $b$  and  $\sigma$  with low regularity or exploding behavior is still an active fields of research.

#### 4.1.4 Sensitivities

If in addition we are interested by computing derivatives of  $u(t, x)$  w.r.t.  $x$  or other model parameters, this is still possible using Monte Carlo simulations. For the sake of simplicity, in our discussion we focus on the gradient of  $u$  w.r.t.  $x$ . Essentially, two approaches are known.

**Resimulation method.** The derivative is approximated using the finite difference method

$$\partial_{x_i} u(t, x) \approx \frac{u(t, x + \varepsilon e_i) - u(t, x - \varepsilon e_i)}{2\varepsilon}$$

where  $e_i = (0, \dots, 0, \underset{i^{th}}{1}, 0, \dots)$ , and  $\varepsilon$  is small. Then, each value function is approximated by its Monte Carlo approximation given in (4.7). However, we have to be careful in generating the Euler scheme starting from  $x + \varepsilon e_i$  and  $x - \varepsilon e_i$ : its sampling should use the same Brownian motion increments, that is

$$\partial_{x_i} u(t, x) \approx \frac{1}{M} \sum_{m=1}^M \frac{\mathcal{E}(f, g, X^{x+\varepsilon e_i, h, m}) - \mathcal{E}(f, g, X^{x-\varepsilon e_i, h, m})}{2\varepsilon}. \quad (4.8)$$

Indeed, for an infinite sample ( $M = +\infty$ ), it does not have any impact on the statistical error whether or not we use the *same driving noise*, but for finite  $M$ , this trick likely maintains a smaller statistical error. Furthermore, the optimal choice of  $h$ ,  $M$  and  $\varepsilon$  is an important issue, but here results are different according to the regularity of  $f$  and  $g$ , we do not go into details.



**Likelihood method.** To avoid the latter problems of selecting the appropriate value of the finite difference parameter  $\varepsilon$ , we may prefer another Monte Carlo estimator of  $\partial_{x_i} u(t, x)$ , which consists in appropriately weighting the output. When  $g$  equals 0, it takes the following form

$$\partial_{x_i} u(t, x) \approx \frac{1}{M} \sum_{m=1}^M f(X_t^{x,h,m}) H_t^{x,h,m} \quad (4.9)$$

where  $H_t^{x,h,m}$  is simultaneously generated with the Euler scheme and does not depend on  $f$ . The advantage of this approach is to avoid the possibly delicate choice of the perturbation parameter  $\varepsilon$  and it is valid for any function  $f$ : thus, it may reduce much the computational time, if many sensitivities are required for the same model. On the other hand, the confidence interval may be larger than that of the resimulation method.

We now provide the formula for the weight  $H$  (known as Bismut-Elworthy-Li formula). It uses the tangent process, which is the (well-defined, see [Kun84]) derivative of  $x \mapsto X_t^x$  w.r.t.  $x$  and which solves

$$DX_t^x := Y_t^x = \text{Id} + \int_0^t Db(X_s^x) Y_s^x ds + \sum_{j=1}^d \int_0^t D\sigma_j(X_s^x) Y_s^x dW_{j,s} \quad (4.10)$$

where  $\sigma_j$  is the  $j$ -th column of the matrix  $\sigma$ .

**Theorem 4.4** *Assume that  $b$  and  $\sigma$  are  $\mathcal{C}_b^2$ -functions, that  $u \in \mathcal{C}^{1,2}([0, T] \times \mathbb{R}^d, \mathbb{R})$  solves the PDE (4.1), and that  $\sigma$  is invertible with a uniformly bounded inverse  $\sigma^{-1}$ . We have*

$$Du(t, x) = \mathbb{E} \left( \frac{f(X_t^x)}{t} \left[ \int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s \right]^\perp \right).$$

PROOF :

First, we recall the decomposition (4.4) obtained from Itô formula, using  $v(s, y) = u(t - s, y)$ :

$$\begin{cases} v(r, X_r^x) = v(0, x) + \int_0^r Dv(s, X_s^x) \sigma(X_s^x) dW_s, & \forall 0 \leq r \leq t, \\ f(X_t^x) = v(t, X_t^x). \end{cases} \quad (4.11)$$

Second, taking expectation, it gives  $v(0, x) = u(t, x) = \mathbb{E}(v(r, X_r^x))$  for any  $r \in [0, T]$ . By differentiating w.r.t.  $x$ , we obtain a nice relation letting the expectation constant in time (actually deeply related to martingale property):

$$Dv(0, x) = \mathbb{E}(Dv(r, X_r^x) Y_r^x), \quad \forall 0 \leq r \leq t.$$

Thus, we deduce

$$\begin{aligned}
Du(t, x) &= Dv(0, x) = \mathbb{E} \left( \frac{1}{t} \int_0^t Dv(s, X_s^x) Y_s^x ds \right) \\
&= \mathbb{E} \left( \frac{1}{t} \left[ \int_0^t Dv(s, X_s^x) \sigma(X_s^x) dW_s \right] \left[ \int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s \right]^\perp \right) \\
&= \mathbb{E} \left( \frac{v(t, X_t^x) - v(0, x)}{t} \left[ \int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s \right]^\perp \right) \\
&= \mathbb{E} \left( \frac{f(X_t^x)}{t} \left[ \int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s \right]^\perp \right)
\end{aligned}$$

using Theorem 3.16 at the second and fourth equality, (4.11) at the third one.  $\square$

In view of the above assumptions of  $u$ , implicitly the function  $f$  is smooth. However, under the current ellipticity condition,  $u$  is still smooth even  $f$  is not; since the formula does depend on  $f$  and not on its derivatives, it is standard to extend the formula to any bounded function  $f$  (without any regularity assumption).

The Monte Carlo evaluation of  $Du(t, x)$  easily follows by independently sampling  $\frac{f(X_t^x)}{t} \left[ \int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s \right]^\perp$  and taking the empirical mean. The exact simulation is not possible and once again, we may use an Euler-type scheme, with time step  $h$ :

- the dimension-augmented Stochastic Differential Equations  $(X^x, Y^x)$  is approximated using the Euler scheme;
- we use a simple-approximation of the stochastic integral

$$\int_0^t [\sigma^{-1}(X_s^x) Y_s^x]^\perp dW_s = \sum_{i=0}^{N-1} [\sigma^{-1}(X_{ih}^{x,h}) Y_{ih}^{x,h}]^\perp (W_{(i+1)h} - W_{ih}).$$

The analysis of discretization error is more intricate than for  $\mathbb{E}(f(X_t^{x,h}) - f(X_t^x))$ : nevertheless, the error is still of magnitude  $h$  (the convergence order is 1 w.r.t.  $h$ , as proved in [GM05c]).

**Theorem 4.5** *Under the setting of Theorem 4.3, for any bounded measurable function  $f$ , we have*

$$\mathbb{E} \left( \frac{f(X_t^{x,h})}{t} \sum_{i=0}^{N-1} \left[ [\sigma^{-1}(X_{ih}^{x,h}) Y_{ih}^{x,h}]^\perp (W_{(i+1)h} - W_{ih}) \right]^\perp \right) - Du(t, x) = O(h).$$

#### 4.1.5 Other theoretical estimates in small time

The representation formula of Theorem 4.4 is the starting point for getting accurate probabilistic estimates on the derivatives of the underlying PDE as time is small, in terms of the fractional smoothness of  $f(X_t^x)$  which is related to the decay of

$$\|f(X_t^x) - \mathbb{E}(f(X_{t-s}^y))\|_{L_2} \quad \text{as } s \rightarrow t.$$

The derivatives are measured in weighted  $L_2$ -norms and surprisingly, the above results are equivalence results [GM10a]; we are not aware of such results using PDE arguments.

**Theorem 4.6** *Under the setting<sup>19</sup> of Theorem 4.3, let  $t$  be fixed, for  $0 < \theta \leq 1$  and a bounded  $f$ , the following assertions are equivalent:*

- i) *for some  $c \geq 0$ ,  $\mathbb{E}|f(X_t^x) - \mathbb{E}(f(X_{t-s}^y))|_{y=X_s^x}|^2 \leq c(t-s)^\theta$  for  $0 \leq s \leq t$ ;*
- ii) *for some  $c \geq 0$ ,  $\mathbb{E}|Du(t-s, X_s^x)|^2 \leq \frac{c}{(t-s)^{1-\theta}}$  for  $0 \leq s < t$ ;*
- iii) *for some  $c \geq 0$ ,  $\int_0^s \mathbb{E}|D^2u(t-r, X_r^x)|^2 dr \leq \frac{c}{(t-s)^{1-\theta}}$  for  $0 \leq s < t$ .*

*If  $0 < \theta < 1$ , it is also equivalent to*

- iv) *for some  $c \geq 0$ ,  $\mathbb{E}|D^2u(t-s, X_s^x)|^2 \leq \frac{c}{(t-s)^{2-\theta}}$  for  $0 \leq s < t$ .*

**Theorem 4.7** *Under the setting of Theorem 4.3, let  $t$  be fixed, for  $0 < \theta < 1$  and a bounded  $f$ , the following assertions are equivalent:*

- i)  $\int_0^t (t-s)^{-\theta-1} \mathbb{E}|f(X_t^x) - \mathbb{E}(f(X_{t-s}^y))|_{y=X_s^x}|^2 ds < +\infty$ ,
- ii)  $\int_0^t (t-s)^{-\theta} \mathbb{E}|Du(t-s, X_s^x)|^2 ds < +\infty$ ,
- iii)  $\int_0^t (t-s)^{1-\theta} \mathbb{E}|D^2u(t-s, X_s^x)|^2 ds < +\infty$ .

## 4.2 The case of Dirichlet boundary conditions and stopped processes

### 4.2.1 Feynman-Kac formula

In view of Corollary 2.5, the natural extension of Theorem 4.1 in the case of Dirichlet boundary condition is the following. We state the result without source term to simplify. The proof is similar and we skip it.

**Theorem 4.8** *Let  $D$  be a bounded domain of  $\mathbb{R}^d$ . Under the setting of Theorem 4.1, assume there is a solution  $u \in \mathcal{C}_b^{1,2}([0, T] \times \overline{D}, \mathbb{R})$  to the PDE*

$$\begin{cases} u'_t(t, x) = L_{b, \sigma\sigma^\perp}^X u(t, x), & \text{for } (t, x) \in ]0, +\infty[ \times D, \\ u(0, x) = f(0, x), & \text{for } x \in D, \\ u(t, x) = f(t, x), & \text{for } (t, x) \in \mathbb{R}^+ \times \partial D, \end{cases} \quad (4.12)$$

*for a given function  $f : \mathbb{R}^+ \times \overline{D} \rightarrow \mathbb{R}$ . Then  $u$  is given by*

$$u(t, x) = \mathbb{E}[f(t - \tau^x \wedge t, X_{\tau^x \wedge t}^x)] \quad (4.13)$$

*for  $x \in D$ , where  $\tau^x = \inf\{s > 0 : X_s^x \notin D\}$  is the first exit time from  $D$  by  $X$ .*

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<sup>19</sup>to simplify the exposure

### 4.2.2 Monte Carlo simulations

Performing a Monte Carlo algorithm in this context is less easy since we have to additionally simulate the exit time of  $X$ . A simple approach consists in discretizing  $X$  using the Euler scheme with time step  $h$ , and then take for the exit time

$$\tau^{x,h} = \inf\{ih > 0 : X_{ih}^{x,h} \notin D\}.$$

It does not require any further computations than those needed to generate  $(X_{ih}^{x,h}, 0 \leq i \leq N)$ . But, the discretization error worsens much since it becomes of magnitude  $\sqrt{h}$ . Actually, even if the values of  $(X_{ih}^{x,h}, 0 \leq i \leq N)$  are generated without error (like in BM case or other simple process), the convergence order is still  $\frac{1}{2}$  w.r.t.  $h$  [Gob00]. The deterioration of the discretization error really comes from the high irregularity of BM paths (and SDE paths): even if two successive points  $X_{ih}^{x,h}$  and  $X_{(i+1)h}^{x,h}$  are close to the boundary but inside the domain, a discrete monitoring scheme does not detect the exit while a continuous BM-like path would likely exit from the domain between  $ih$  and  $(i+1)h$ . Moreover, it gives a systematic (in mean) underestimation of the true exit time. To overcome this lack of accuracy, there are several improved schemes.

- The Brownian bridge technique consists in simulating the exit time of local arithmetic BM (corresponding to the local dynamics of Euler scheme, see 1.12). For simple domain like half-space, the procedure is explicit and tractable, this is related the explicit knowledge of the distribution of the Brownian maximum, see Proposition 1.9. For smooth domain, we can approximate locally the domain by half-spaces. This improvement allows to recover the order 1 for the convergence, see [Gob00] and [Gob01]. For non smooth domains (including corners for instance) and general SDEs, providing an accurate scheme and performing its error analysis is still an open issue; for heuristics and numerical experiments, see [Gob09] for instance.
- The boundary shifting method consists in shrinking the domain to compensate the systematic bias in the simulation of the discrete exit time. Very remarkably, there is an universal elementary rule to make the domain smaller:

*locally at a point  $y$  close to the boundary, move the boundary  
inwards by a quantity proportional to  $c_0\sqrt{h}$  times  
the norm of the diffusion coefficient in the normal direction.*

The constant  $c_0$  is equal to the mean of the asymptotic overshoot of the Gaussian random walk as the ladder height goes to infinity: it can be expressed using the zeta function

$$c_0 = -\frac{\zeta(\frac{1}{2})}{\sqrt{2\pi}} = 0.5826 \dots$$

This procedure strictly improves the order  $\frac{1}{2}$  of the discrete procedure, but it is still an open question whether the convergence order is 1, although numerical experiments corroborates this fact.

The result is stated as follows, see [GM10b].

**Theorem 4.9** *Assume that the domain  $D$  is bounded and has a  $C^3$ -boundary, that  $b, \sigma$  are  $C_b^2$  and  $f \in C_b^{1,2}$ . Let  $n(y)$  be the unit inward normal vector to the boundary  $\partial D$  at the closest<sup>20</sup> point to  $y$  on the boundary. Set*

$$\hat{\tau}^{x,h} = \inf \{ih > 0 : X_{ih}^{x,h} \notin D \text{ or } d(X_{ih}^{x,h}, \partial D) \leq c_0 \sqrt{h} |n^\perp \sigma|(X_{ih}^{x,h})\}.$$

Then, we have

$$\mathbb{E}[f(t - \hat{\tau}^{x,h} \wedge t, X_{\hat{\tau}^{x,h} \wedge t}^x)] - \mathbb{E}[f(t - \tau^x \wedge t, X_{\tau^x \wedge t}^x)] = o(\sqrt{h}).$$

Observe that this improvement is very cheap regarding the computational cost. It can be extended (regarding to the numerical scheme and its mathematical analysis) to a source term, to time-dependent domain and to stationary problems (elliptic PDE).

**Complementary references:** see [CDL<sup>+</sup>89], [Sab91], [KP95], [LPS98], [Gla03], [AG07] for general references. For reflected processes and Neumann boundary conditions, see [Gob01] and [BGT04]. For variance reduction techniques, see [New94], [GM05a] and [JL09]. For domain decomposition, see [PT03] and [GM05b]. This list is not exhaustive.

## 5 Backward stochastic differential equations and semi-linear PDEs

The link between PDEs and stochastic processes have been developed since several decades and more recently, say in the last twenty years, researchers have paid attention to the probabilistic interpretation of non-linear PDEs, and in particular semi-linear PDEs. These PDEs are connected to non-linear processes, called Backward Stochastic Differential Equations (BSDE in short). In this section, we define these equations, firstly introduced by Pardoux and Peng [PP90], and give their connection with PDEs. Finally, we present a Monte Carlo algorithm to simulate them, using empirical regressions: it has the advantage to suit well the case of multidimensional problems, with a great generality on the type of semi-linearity.

These equations have many fruitful applications in stochastic control theory and mathematical finance, where they usually provide elegant proofs to characterize the solution to optimal decision problems for instance. For the applications, we refer to reader to [EPQ97] and [EHM08] for instance.

### 5.1 Existence of BSDE and Feynman-Kac formula

#### 5.1.1 Heuristics

As a difference with a Stochastic Differential Equation defined by (3.21) where the initial condition is given and the dynamics is imposed, a Backward SDE is defined through a

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<sup>20</sup>uniquely defined if  $y$  is close to the boundary

random *terminal condition*  $\xi$  at a fixed terminal  $T$  and a dynamics imposed by a *driver*  $g$ . It takes the form

$$Y_t = \xi + \int_t^T g(s, Y_s, Z_s) ds - \int_t^T Z_s dW_s \quad (5.1)$$

where we write the integrals between  $t$  and  $T$  to emphasize on the backward point of view:  $\xi$  should be thought as a stochastic target to reach at time  $T$ . A solution to (5.1) is the couple  $(Y, Z)$ : without extra conditions, the problem has an infinite number of solutions and thus is ill-posed. For instance, if  $g \equiv 0$  and  $\xi = f(W_T)$ : taking  $c \in \mathbb{R}$ , a solution is  $Z_t = c$  and  $Y_t = \xi + c(W_T - W_t)$ , thus uniqueness fails. In addition to integrability properties (appropriate  $L_2$ -spaces) that we do not detail, an important condition is that the solution does not anticipate the future of BM, i.e. the solution  $Y_t$  depends on the Brownian Motion  $W$  up to  $t$ , and similarly to  $Z$ : we informally say that *the solution is adapted to  $W$* . In a stochastic control problem, this adaptedness constraint is natural since it states that the value function or the decision can not be made in advance to the flow of information given by  $W$ . Observe that in the uniqueness counter-example,  $Y$  is not adapted to  $W$  since  $Y_t$  depends on the BM on  $[0, T]$  and not only on  $[0, t]$ .

Taking the conditional expectation in (5.1) gives

$$Y_t = \mathbb{E}\left(\xi + \int_t^T g(s, Y_s, Z_s) ds \mid W_s : s \leq t\right), \quad (5.2)$$

because the stochastic integral (built with Brownian increments after  $t$ ) is centered conditionally on the BM up to time  $t$ . Of course, this rule is fully justified by the stochastic calculus theory. Since  $Y_t$  in (5.2) is adapted to  $W$ , it should be the right solution (if unique); then,  $Z$  serves as a control to make the equation (5.1) valid (with  $Y$  adapted).

### 5.1.2 Feynman-Kac formula

The connection with PDE is possible when the terminal condition is a function of a (forward) SDE: this case is called *Markovian BSDE*. Additionally, the driver may depend also on this SDE as  $g(s, X_s, Y_s, Z_s)$  for a deterministic function  $g$ . We now state by a verification theorem. To allow a more natural presentation as backward system, we choose to write the semi-linear PDE with a terminal condition at time  $T$  instead of an initial condition at time 0.

**Theorem 5.1** *Let  $T > 0$  be given. Under the assumptions of Theorem 3.17, let  $X^x$  be the solution (3.21) starting from  $x \in \mathbb{R}^d$ , assume there is a solution  $v \in \mathcal{C}_b^{1,2}([0, T] \times \mathbb{R}^d, \mathbb{R})$  to the semi-linear PDE*

$$\begin{cases} v'_t(t, x) + L_{b, \sigma \sigma^\perp}^X v(t, x) + g(t, x, v(t, x), Dv(t, x) \sigma(x)) = 0, \\ v(T, x) = f(x), \end{cases} \quad (5.3)$$

*for two given functions  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  and  $g : [0, T] \times \mathbb{R}^d \times \mathbb{R} \times (\mathbb{R} \otimes \mathbb{R}^d) \rightarrow \mathbb{R}$ . Then,  $Y_t^x = v(t, X_t^x)$  and  $Z_t^x = [Dv \sigma](t, X_t^x)$  solves the BSDE*

$$Y_t^x = f(X_T^x) + \int_t^T g(s, X_s^x, Y_s^x, Z_s^x) ds - \int_t^T Z_s^x dW_s. \quad (5.4)$$

PROOF :

The Itô formula (4.3) applied to  $v$  and the  $X^x$  gives

$$\begin{aligned} dv(s, X_s^x) &= [v'_s(s, X_s^x) + L_{b, \sigma \sigma^\perp}^X v(s, X_s^x)] ds + Dv(s, X_s^x) \sigma(X_s^x) dW_s \\ &= -g(s, X_s^x, v(s, X_s^x), [Dv \sigma](s, X_s^x)) ds + Dv(s, X_s^x) \sigma(X_s^x) dW_s, \end{aligned}$$

which writes between  $s = t$  and  $s = T$ :

$$v(T, X_T^x) = v(t, X_t^x) - \int_t^T g(s, X_s^x, v(s, X_s^x), [Dv \sigma](s, X_s^x)) ds + \int_t^T Dv(s, X_s^x) \sigma(X_s^x) dW_s.$$

Since  $v(T, \cdot) = f(\cdot)$ , we complete the proof by identification.  $\square$

In particular, at time 0 where  $X_0^x = x$ , we obtain  $Y_0^x = v(0, x)$  and in view of (5.2), it gives a Feynman-Kac representation to  $v$ :

$$v(0, x) = \mathbb{E} \left( f(X_T^x) + \int_t^T g(s, X_s^x, Y_s^x, Z_s^x) ds \right). \quad (5.5)$$

As in case of linear PDEs, the assumption of uniform smoothness on  $v$  up to  $T$  is too strong to include the case of non-smooth terminal function  $f$ . But with an extra ellipticity condition, as for the heat equation, the solution becomes smooth immediately away from  $T$  (see [Fri64]) and a similar verification could be checked under milder conditions.

The above Backward SDE (5.4) is coupled to a Forward SDE, but the latter is not coupled to the BSDE. Another interesting extension is to allow the coupling in both directions by having the coefficients of  $X$  dependent on  $v$ , i.e.  $b(x)$  and  $\sigma(x)$  become functions of  $x, v(t, x), Dv(t, x)$ . The resulting process is called a Forward Backward Stochastic Differential Equations and is related to Quasi-Linear PDEs, where the operator  $L_{b, \sigma \sigma^\perp}^X$  also depends on  $v$  and  $Dv$ , see [MY99].

### 5.1.3 Other existence results without PDE framework

So far, only Markovian BSDEs are presented but from the probabilistic point of view, the Markovian structure is not required to define a solution: what is really crucial is the ability to represent a random variable built from  $(W_s : s \leq T)$  as a stochastic integral w.r.t. the Brownian motion. This point has been discussed in Corollary 3.7. Then, in the simple case where  $g$  is Lipschitz w.r.t.  $y, z$ ,  $(Y, Z)$  are built by means of a usual fixed point procedure in suitable  $L_2$ -norms and of this stochastic integral representation. We now state a more general existence and uniqueness result for BSDE, which is valid without any underlying (finite-dimensional) semi-linear PDE, we omit the proof.

**Theorem 5.2** *Let  $T > 0$  be fixed and assume the assumptions of Theorem 3.17 for the existence of  $X$  and that*

- *the terminal condition  $\xi = f(X_s : s \leq T)$  is a square integrable functional of the SDE  $(X_s : s \leq T)$ ;*

- the measurable function  $g : [0, T] \times \mathbb{R}^d \times \mathbb{R} \times (\mathbb{R} \otimes \mathbb{R}^d)$  is uniformly Lipschitz in  $(y, z)$ :

$$|g(t, x, y_1, z_1) - g(t, x, y_2, z_2)| \leq C_g(|y_1 - y_2| + |z_1 - z_2|),$$

uniformly in  $(t, x)$ ;

- the driver is square integrable at  $(y, z) = (0, 0)$ :  $\mathbb{E}(\int_0^T g^2(t, X_t, 0, 0)dt) < +\infty$ .

Then, there exists a unique solution  $(Y, Z)$ , adapted and in  $L_2$ -spaces, to

$$Y_t = f(X_s : s \leq T) + \int_t^T g(s, X_s, Y_s, Z_s)ds - \int_t^T Z_s dW_s.$$

Many works have been done in the last decade to go beyond the case of Lipschitz driver, which may be too stringent for some applications. In particular, having  $g$  with quadratic growth in  $Z$  is particularly interesting in exponential utility maximization problem (the non-linear PDE term is quadratic in  $|Dv|$ ). This leads to quadratic BSDEs (see for instance [Kob00]). A simple example of such BSDEs can be cooked up from heat equation and Brownian motion. Namely from Corollary 3.7, for a smooth function  $f$  with compact support, set  $u(t, x) = \mathbb{E}(\exp(f(x + W_t)))$  and  $v(t, y) = u(1 - t, y)$ , so that

$$\begin{aligned} \exp(f(W_1)) &= u(1, 0) + \int_0^1 u'_x(1 - s, W_s) dW_s, \\ u(1 - t, W_t) &= u(1, 0) + \int_0^t u'_x(1 - s, W_s) dW_s, \\ v(t, W_t) &= \exp(f(W_1)) - \int_t^1 v'_x(s, W_s) dW_s, \end{aligned}$$

and by setting  $Y_t = \log(v(t, W_t))$  and  $Z_t = v'_x(t, W_t)/Y_t$ , we obtain

$$Y_t = f(W_1) + \int_t^1 \frac{1}{2} Z_s^2 ds - \int_t^1 Z_s dW_s,$$

which is the simplest quadratic BSDE.

## 5.2 Time discretization and dynamic programming equation

### 5.2.1 Explicit and implicit schemes

To perform the simulation, a first stage may be the derivation of a discretization scheme, written backwardly in time (*backward dynamic programming equation*). For the further analysis, assume that the terminal condition is of the form  $\xi = f(X_T)$  where  $X$  is standard (forward) SDE.

Consider a time grid with  $N$  time steps  $\pi = \{0 = t_0 < \dots < t_i < \dots < t_N = T\}$ , with possibly non uniform time step, and set  $|\pi| = \max_i(t_{i+1} - t_i)$ . We will suppose later that  $|\pi| \rightarrow 0$ .



We write  $\Delta_i = t_{i+1} - t_i$  and  $\Delta W_i = W_{t_{i+1}} - W_{t_i}$ . Writing the equation (5.4) between times  $t_i$  and  $t_{i+1}$ , we have

$$Y_{t_i} = Y_{t_{i+1}} + \int_{t_i}^{t_{i+1}} g(s, X_s, Y_s, Z_s) ds - \int_{t_i}^{t_{i+1}} Z_s dW_s.$$

Then, by applying simple approximations for  $ds$  and  $dW_s$  integrals and by replacing  $X$  by a Euler scheme computed along the grid  $\pi$  (and denoted  $X^\pi$ ), we may define the discrete BSDE as

$$(Y_{t_i}^\pi, Z_{t_i}^\pi) = \arg \min_{(Y, Z) \in L_2(\mathcal{F}_{t_i}^\pi)} \mathbb{E}(Y_{t_{i+1}}^\pi + \Delta_i g(t_i, X_{t_i}^\pi, Y, Z) - Y - Z \Delta W_i)^2$$

with the initialization  $Y_T^\pi = f(X_T^\pi)$  at  $i = N$ , where  $L_2(\mathcal{F}_{t_i}^\pi)$  stands for the set of random variables (with appropriate dimension) that are square integrable and depend on the Brownian motion increments  $(\Delta W_j : j \leq i - 1)$ . The latter property is the measurability w.r.t. the sigma fields  $\mathcal{F}_{t_i}^\pi$  generated by  $(\Delta W_j : j \leq i - 1)$ .

Then, a direct computation using the properties of Brownian increments gives

$$\begin{cases} Y_T^\pi = f(X_T^\pi), \\ Z_{t_i}^\pi = \frac{1}{\Delta_i} \mathbb{E}(Y_{t_{i+1}}^\pi \Delta W_i^\perp | \mathcal{F}_{t_i}^\pi), & i < N \\ Y_{t_i}^\pi = \mathbb{E}(Y_{t_{i+1}}^\pi + \Delta_i g(t_i, X_{t_i}^\pi, Y_{t_i}^\pi, Z_{t_i}^\pi) | \mathcal{F}_{t_i}^\pi), & i < N. \end{cases} \quad (5.6)$$

This is the *implicit scheme* since the arguments of the function at the r.h.s. depend on the quantity  $Y_{t_i}^\pi$  to compute on the l.h.s. Nevertheless, since  $g$  is uniformly Lipschitz in  $y$ , it is not difficult to show that the Dynamic Programming Equation (DPE in short) (5.6) is well-defined for  $|\pi|$  small enough and that  $Y_{t_i}^\pi$  can be computed using a Picard iteration procedure.

It is easy to turn the previous scheme into an explicit scheme and therefore, to avoid this extra Picard procedure. It writes

$$\begin{cases} Y_T^\pi = f(X_T^\pi), \\ Z_{t_i}^\pi = \frac{1}{\Delta_i} \mathbb{E}(Y_{t_{i+1}}^\pi \Delta W_i^\perp | \mathcal{F}_{t_i}^\pi), & i < N \\ Y_{t_i}^\pi = \mathbb{E}(Y_{t_{i+1}}^\pi + \Delta_i g(t_i, X_{t_i}^\pi, Y_{t_{i+1}}^\pi, Z_{t_i}^\pi) | \mathcal{F}_{t_i}^\pi), & i < N. \end{cases} \quad (5.7)$$

In our personal experience on numerics, we have not observed a significant outperformance of one scheme on another. Moreover, from the theoretical point of view, both schemes exhibit the same rates of convergence w.r.t.  $|\pi|$ , at least when the driver is Lipschitz.

The explicit scheme is the simplest one, and this is the one that we recommend in practice.

### 5.2.2 Time discretization error

Define the measure of the quadratic error

$$\mathcal{E}(Y^\pi - Y, Z^\pi - Z) = \max_{0 \leq i \leq N} \mathbb{E}|Y_{t_i}^\pi - Y_{t_i}|^2 + \sum_{i=0}^{N-1} \int_{t_i}^{t_{i+1}} \mathbb{E}|Z_{t_i}^\pi - Z_t|^2 dt.$$

Although not explicitly mentioned in the previous existence results on BSDE, this type of norm is appropriate to perform the fixed point argument in the proof of Theorem 5.2. We now state an error estimate [GL06], in order to show the convergence of the DPE to the BSDE.

**Theorem 5.3** *For a Lipschitz driver w.r.t.  $(x, y, z)$  and  $\frac{1}{2}$ -Hölder w.r.t.  $t$ , there is a constant  $C$  independent on  $\pi$  such that we have*

$$\begin{aligned} \mathcal{E}(Y^\pi - Y, Z^\pi - Z) \leq & C \left( |\pi| + \sup_{i \leq N} \mathbb{E}|X_{t_i}^\pi - X_{t_i}|^2 + \mathbb{E}|f(X_T^\pi) - f(X_T)|^2 \right. \\ & \left. + \sum_{i=0}^{N-1} \frac{1}{\Delta_i} \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} \mathbb{E}|Z_t - Z_s|^2 ds dt \right). \end{aligned}$$

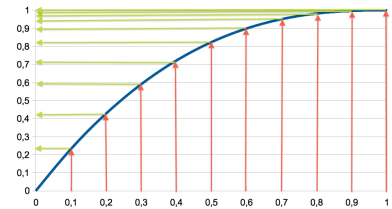
Let us discuss on the nature and the magnitude of different error contributions.

- First, we face the *strong approximation error* of the forward SDE by its Euler scheme. Here we rather focus on convergence of paths (in  $L_2$ -norms), whereas in Paragraph 4.1.3, we have studied the convergence of expectations of function of  $X_T^\pi$  towards those of  $X_T$ . Anyway, the problem is now well-understood: under Lipschitz condition on  $b$  and  $\sigma$ , we can prove  $\sup_{i \leq N} \mathbb{E}|X_{t_i}^\pi - X_{t_i}|^2 = O(|\pi|)$ .
- Second, we should ensure a good *strong approximation* of the terminal conditions: if  $f$  is Lipschitz continuous, it readily follows from the previous term and  $\mathbb{E}|f(X_T^\pi) - f(X_T)|^2 = O(|\pi|)$ . For non Lipschitz  $f$ , there are partial answers, see [Avi09].
- Finally, the last contribution  $\sum_{i=0}^{N-1} \frac{1}{\Delta_i} \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} \mathbb{E}|Z_t - Z_s|^2 ds dt$  is related to the  $L_2$ -regularity of  $Z$  and is intrinsic to the BSDE-solution. For smooth data,  $Z$  has the same regularity of Brownian paths and this error term is  $O(|\pi|)$ . For non smooth  $f$  (but under ellipticity condition on  $X$ ), the  $L_2$ -norm of  $Z_t$  blows up as  $t \rightarrow T$  and the rate  $|\pi|$  usually worsens: for instance for  $f(x) = 1_{x \geq 0}$ , it becomes  $N^{-\frac{1}{2}}$  for uniform time-grid.

The analysis is very closely related to the fractional smoothness of  $f(X_T)$  briefly discussed in Paragraph 4.1.5, see also [GGG12]. Choosing an appropriate grid of the form

$$t_k^{\bar{\theta}} = T - T(1 - k/N)^{1/\bar{\theta}} \quad (\bar{\theta} \in (0, 1])$$

compensates this blow-up (for appropriate value of  $\bar{\theta}$ ) and enables to retrieve the rate  $N^{-1}$ .



On the horizontal axis, uniform grid. On the vertical axis, the grid  $(t_k^{\bar{\theta}} : 0 \leq k \leq N)$ .  $T = 1$ .

Actually in [GL07], it is shown that the upper bounds in Theorem 5.3 can be refined for smooth data, to finally obtain that the main error comes from *strong approximation error* on the forward component. This is an incentive to accurately approximate the SDE in  $L_2$ -sense.

### 5.2.3 Towards the resolution of the Dynamic Programming Equation

The effective implementation of the explicit scheme (5.7) requires the iterative computations of conditional expectations: this is discussed in the next paragraphs.

Prior to this, we make some preliminary simplifications. Actually it can be easily seen that it is enough to take the conditioning w.r.t.  $X_{t_i}^\pi$  instead of  $\mathcal{F}_{t_i}^\pi$ , because of the Markovian property of  $X^\pi$  along the grid  $\pi$  and of the independent Brownian increments. Thus, (5.7) becomes

$$\begin{cases} Y_T^\pi = f(X_T^\pi), \\ Z_{t_i}^\pi = \frac{1}{\Delta_i} \mathbb{E}(Y_{t_{i+1}}^\pi \Delta W_i^\perp | X_{t_i}^\pi), & i < N \\ Y_{t_i}^\pi = \mathbb{E}(Y_{t_{i+1}}^\pi + \Delta_i g(t_i, X_{t_i}^\pi, Y_{t_{i+1}}^\pi, Z_{t_i}^\pi) | X_{t_i}^\pi), & i < N. \end{cases} \quad (5.8)$$

The same arguments apply to assert that for some (measurable) deterministic functions  $y_i^\pi$  and  $z_i^\pi$  we have

$$y_i^\pi(X_{t_i}^\pi) = Y_{t_i}^\pi, \quad z_i^\pi(X_{t_i}^\pi) = Z_{t_i}^\pi. \quad (5.9)$$

Therefore, computing  $(Y^\pi, Z^\pi)$  is equivalent to the computation of  $y_i^\pi$  and  $z_i^\pi$ , for any  $i$ .

## 5.3 Approximation of conditional expectations using least-squares method

### 5.3.1 Empirical least-squares problem

We adopt the point of view of conditional expectation as a *projection operator in  $L_2$* . This is not the only possible approach, but it has the advantage (as it will be seen later)

1. to be much flexible w.r.t. the knowledge on the model for  $X$  (or  $X^\pi$ ): only independent simulations of  $X^\pi$  are required (which is straightforward to perform);
2. to be little demanding on the assumptions on the underlying stochastic model: in particular, no ellipticity nor degeneracy condition are required, it could also include jumps (corresponding to PDE with a non-local Integro-Differential operator);
3. to provide robust theoretical error estimates, which allow to optimally tune the convergence parameters;
4. to be possibly adaptive to the data (*data-driven* scheme).

We recall that if a scalar random variable  $R$  (called the *response*) is square integrable, the conditional expectation of  $R$  given another possibly multidimensional r.v.  $O$  (called the *observation*) is given by

$$\mathbb{E}(R|O) = \underset{m(O) \text{ s.t. } m(\cdot) \text{ is a meas. funct. with } \mathbb{E}|m(O)|^2 < +\infty}{\text{Arg min}} \mathbb{E}|R - m(O)|^2.$$

This is a least-squares problem in infinite dimension, also called *regression problem*. Usually in this context of BSDE simulation, none of the distributions of  $O$ ,  $R$  or  $(O, R)$  is

known in analytical and tractable form: thus an exact computation of  $\mathbb{E}(R|O)$  is hopeless. The difficulty remains unchanged if we approximate the regression function

$$m(\cdot) = \mathbb{E}(R|O = \cdot)$$

on a finite dimensional functions basis. Alternatively, we can rely on independent simulations of  $(O, R)$  to compute an empirical version of  $m$ . This is the approach subsequently developed.

The functions basis are  $(\phi_k(\cdot))_{1 \leq k \leq K}$  and we assume that  $\mathbb{E}|\phi_k(O)|^2 < +\infty$  for any  $k$ . We emphasize that

we can not assume that  $(\phi_k(O))_{1 \leq k \leq K}$  forms an orthonormal basis functions in  $L_2$ , since in our setting, the distribution of  $O$  is not explicit. Using this finite dimensional approximation, we anticipate to unfortunately retrieve the curse of dimensionality: the larger the dimension  $d$  of  $O$ , the larger the required  $K$  for a good accuracy of  $m$ , the larger the complexity.

We compute the coefficients on the basis by solving a *empirical least-squares problem*

$$(\alpha_k^M)_k = \arg \min_{\alpha \in \mathbb{R}^K} \frac{1}{M} \sum_{i=1}^M (R_i - \sum_{k=1}^K \alpha_k \phi_k(O_i))^2,$$

where  $(R_i, O_i)_{1 \leq i \leq M}$  are independent simulations of the couple  $(R, O)$ . Then, for the approximation of  $m$ , we set

$$\tilde{m}_M(\cdot) = \sum_{k=1}^K \alpha_k^M \phi_k(\cdot).$$

To efficiently compute the coefficients  $(\alpha_k^M)_k$ , we might use a SVD decomposition to account for instability issues, see [GL96].

### 5.3.2 Model-free error estimates

Without extra assumptions on the model, we can derive model-free error estimates, see [GKKW02].

**Theorem 5.4** *Assume that*

- $R = m(O) + \epsilon$  with  $\mathbb{E}(\epsilon|X) = 0$ ,<sup>21</sup>
- $(O_1, R_1), \dots, (O_M, R_M)$  are independent copies of  $(O, R)$ ;
- $\sigma^2 = \sup_x \text{Var}(R|O = x) < +\infty$ ;
- $\Phi = \text{Span}(\phi_1, \dots, \phi_K)$  is a linear vector space of dimension  $K$ .

Denote by  $\mu^M$  the empirical measure associated to  $(O_1, \dots, O_M)$ ,  $\mu$  the probability measure of  $O$  and by  $|\phi|_M^2 = \frac{1}{M} \sum_{i=1}^M \phi^2(O_i)$  the empirical  $L_2$ -measure of  $\phi$  w.r.t.  $\mu^M$ , and set

$$\tilde{m}_M(\cdot) = \arg \min_{\phi \in \Phi} \frac{1}{M} \sum_{i=1}^M |\phi(O_i) - R_i|^2. \quad (5.10)$$

---

<sup>21</sup>meaning that  $m(O) = \mathbb{E}(R|O)$ .

Then

$$\mathbb{E}(|\tilde{m}_M - m|_M^2) \leq \sigma^2 \frac{K}{M} + \min_{\phi \in \Phi} |\phi - m|_{L_2(\mu)}^2.$$

The first term in the r.h.s. above is interpreted as a *statistical error*<sup>22</sup> term (due to a finite sample to compute the empirical coefficients), while the second term is an *approximation error of function class*<sup>23</sup> (due to finite-dimensional vector space). The first term converges to 0 as  $M \rightarrow +\infty$  but it blows up if  $K \rightarrow +\infty$ , while the second one converges to 0 as  $K \rightarrow +\infty$  (as least if  $\Phi$  asymptotically spans all the functions in  $L_2(\mu)$ ). This bias-variance decomposition shows that there is a necessary trade-off between  $K$  and  $M$  to ensure a convergent approximation. Without this right balance, the approximation (5.10) may be not convergent. Furthermore, the parameter tuning can also be made optimally.

In the quoted reference [GKKW02], the space  $\Phi$  could also depend on the simulations (data-driven approximation spaces).

PROOF :

Assume that

$$\mathbb{E}\left(|\tilde{m}_M - m|_M^2 | O_1, \dots, O_M\right) \leq \sigma^2 \frac{K}{M} + \min_{\phi \in \Phi} |\phi - m|_M^2. \quad (5.11)$$

Then, the announced result directly follows by taking expectations and observing that

$$\mathbb{E}\left(\min_{\phi \in \Phi} |\phi - m|_M^2\right) \leq \min_{\phi \in \Phi} \mathbb{E}\left(|\phi - m|_M^2\right) = \min_{\phi \in \Phi} |\phi - m|_{L_2(\mu)}^2.$$

We now prove (5.11). As far as computations conditionally on  $O_1, \dots, O_M$  are concerned, without loss of generality we can assume that  $(\phi_1, \dots, \phi_{K_M})$  is an orthonormal family in  $L_2(\mu^M)$ , with possibly  $K_M \leq K$ :  $\frac{1}{M} \sum_{i=1}^M \phi_k(O_i) \phi_l(O_i) = \delta_{k,l}$ . Consequently, the solution

$\arg \min_{\phi \in \Phi} \frac{1}{M} \sum_{i=1}^M |\phi(O_i) - R_i|^2$  is given by

$$\tilde{m}_M(\cdot) = \sum_{j=1}^{K_M} \alpha_j \phi_j(\cdot) \quad \text{with} \quad \alpha_j = \frac{1}{M} \sum_{i=1}^M \phi_j(O_i) R_i.$$

Now, set  $\mathbb{E}^*(\cdot) = \mathbb{E}(\cdot | O_1, \dots, O_M)$ . Then, observe that  $\mathbb{E}^*(\tilde{m}_M(\cdot))$  is the least-squares solution to  $\min_{\phi \in \Phi} \frac{1}{M} \sum_{i=1}^M |\phi(O_i) - m(O_i)|^2 = \min_{\phi \in \Phi} |\phi - m|_M^2$ . Indeed,

- on the one hand, the above least-squares solution is given by  $\sum_{j=1}^{K_M} \alpha_j^* \phi_j(\cdot)$  with  $\alpha_j^* = \frac{1}{M} \sum_{i=1}^M \phi_j(O_i) m(O_i)$ ;
- on the other hand,  $\mathbb{E}^*(\tilde{m}_M(\cdot)) = \sum_{j=1}^{K_M} \mathbb{E}^*(\alpha_j) \phi_j(\cdot)$  and  $\mathbb{E}^*(\alpha_j) = \frac{1}{M} \sum_{i=1}^M \phi_j(O_i) \mathbb{E}^*(R_i) = \frac{1}{M} \sum_{i=1}^M \phi_j(O_i) \mathbb{E}(m(O_i) + \epsilon_i | O_1, \dots, O_M) = \alpha_j^*$ .

Thus, by the Pythagoras theorem, we obtain

$$\begin{aligned} |\tilde{m}_M - m|_M^2 &= |\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 + |\mathbb{E}^*(\tilde{m}_M) - m|_M^2, \\ \mathbb{E}^*|\tilde{m}_M - m|_M^2 &= \mathbb{E}^*|\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 + |\mathbb{E}^*(\tilde{m}_M) - m|_M^2 \\ &= \mathbb{E}^*|\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 + \min_{\phi \in \Phi} |\phi - m|_M^2. \end{aligned}$$

---

<sup>22</sup>also called variance term.

<sup>23</sup>squared bias term.

Since  $(\phi_j)_j$  is orthonormal in  $L_2(\mu_M)$ , we have  $|\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 = \sum_{j=1}^{K_M} |\alpha_j - \mathbb{E}^*(\alpha_j)|^2$ . Since  $\alpha_j - \mathbb{E}^*(\alpha_j) = \frac{1}{M} \sum_{i=1}^M \phi_j(O_i)(R_i - m(O_i))$ , we obtain

$$\begin{aligned} \mathbb{E}^*|\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 &= \sum_{j=1}^{K_M} \frac{1}{M^2} \mathbb{E}^* \sum_{i,l=1}^M \phi_j(O_i) \phi_j(O_l) (R_i - m(O_i))(R_l - m(O_l)) \\ &= \sum_{j=1}^{K_M} \frac{1}{M^2} \sum_{i=1}^M \phi_j^2(O_i) \text{Var}(R_i|O_i) \end{aligned}$$

taking advantage that the  $(\epsilon_i)_i$  conditionally on  $(O_1, \dots, O_M)$  are centered. This proves

$$\mathbb{E}^*|\tilde{m}_M - \mathbb{E}^*(\tilde{m}_M)|_M^2 \leq \sigma^2 \sum_{j=1}^{K_M} \frac{1}{M^2} \sum_{i=1}^M f_j^2(O_i) = \sigma^2 \frac{K_M}{M} \leq \sigma^2 \frac{K}{M}.$$

The proof of (5.11) is complete.  $\square$

### 5.3.3 Least-Squares method for solving discrete BSDE

We now apply the previous empirical least-squares method to numerically solve the DPE (5.8). To alleviate the presentation and to avoid some unimportant technicalities, we directly assume that the terminal condition  $f(\cdot)$  is Lipschitz bounded and the driver at zero  $((t, x) \mapsto g(t, x, 0, 0))$  as well. For simplicity of exposure, we consider here only uniform time grids with  $N$  time steps.

**Proposition 5.5** *Under these assumptions, the functions  $y_i^\pi(\cdot)$  and  $\sqrt{N}z_i^\pi(\cdot)$  defined in (5.9) are Lipschitz continuous and bounded: their Lipschitz constants and upper bounds are denoted by  $C_\star$ , which can be taken independent on  $N$  and  $i$ .*

Actually,  $C_\star$  can be given explicitly in terms of the data.

For more important reasons, we consider a slightly variant of (5.8) where the Brownian increments are truncated at level  $R_w \sqrt{T/N}$  where  $R_w > 0$  is large enough: for this we use the notation

$$[\Delta W_k]_w = \left( -R_w \sqrt{\frac{T}{N}} \vee \Delta W_{1,k} \wedge R_w \frac{T}{N}, \dots, -R_w \sqrt{\frac{T}{N}} \vee \Delta W_{d,k} \wedge R_w \sqrt{\frac{T}{N}} \right).$$

The DPE is now

$$\begin{cases} Y_T^{\pi, R_w} = f(X_T^\pi), \\ Z_{t_i}^{\pi, R_w} = \frac{1}{\Delta_i} \mathbb{E}(Y_{t_{i+1}}^{\pi, R_w} [\Delta W_i]_w^\perp | X_{t_i}^\pi), \quad i < N \\ Y_{t_i}^{\pi, R_w} = \mathbb{E}(Y_{t_{i+1}}^{\pi, R_w} + \Delta_i g(t_i, X_{t_i}^\pi, Y_{t_{i+1}}^{\pi, R_w}, Z_{t_i}^{\pi, R_w}) | X_{t_i}^\pi), \quad i < N. \end{cases} \quad (5.12)$$

The  $L_2$ -error between  $(Y^\pi, Z^\pi)$  and  $(Y^{\pi, R_w}, Z^{\pi, R_w})$  is exponentially small w.r.t.  $R_w$ , because of Gaussian type inequalities for the tails of  $\Delta W_i$ : thus, a choice like  $R_w = c \log(N)$  for  $c$  large enough provides an extra error which can be neglected in comparison to the discretization error. We will explain later in which sense this truncation is useful. This truncation does not modify the statement of Proposition 5.5 for  $y_i^{\pi, R_w}(\cdot)$  and  $\sqrt{N}z_i^{\pi, R_w}(\cdot)$ , for which the Lipschitz and boundedness properties are still valid with the same constant  $C_\star$ .

**Algorithm for approximating of  $y_k^{\pi, R_w}(\cdot)$  and  $z_k^{\pi, R_w}(\cdot)$**  At each time index  $0 \leq k \leq N - 1$ , we consider basis functions  $p_{0,k}(\cdot)$  for the  $y_k^{\pi, R_w}$ -component and  $p_{l,k}(\cdot)$  for the  $l$ -th component of  $z_k^{\pi, R_w}$  ( $1 \leq l \leq d$ ). These basis functions are understood as vectors of functions, with size  $K_{0,k}$  and  $K_{l,k}$  respectively. The final approximation of  $y_k^{\pi, R_w}(\cdot)$  and  $z_k^{\pi, R_w}(\cdot)$  have the form

$$y_k^{\pi, R_w, M}(\cdot) = [\alpha_{0,k}^M \cdot p_{0,k}(\cdot)]_y, \quad z_{l,k}^{\pi, R_w, M}(\cdot) = [\alpha_{l,k}^M \cdot p_{l,k}(\cdot)]_z,$$

where  $[\psi]_y = -C_\star \vee \psi \wedge C_\star$  and  $[\psi]_z = -C_\star N^{1/2} \vee \psi \wedge C_\star N^{1/2}$  truncate the solution at the same threshold as the exact solution. The coefficients  $\alpha_{l,k}^M$  ( $0 \leq l \leq d$ ) are computed with  $M$  independent simulations of  $(X_{t_k}^\pi)_k$  and  $(\Delta W_k)_k$ , that are denoted by  $\{(X_{t_k}^{\pi, m})_k\}_{1 \leq m \leq M}$  and  $\{(\Delta W_k^m)_k\}_{1 \leq m \leq M}$ : this single set of simulated paths are used to compute all the coefficients at once. This is done as follows.

▷ Initialization : for  $k = N$ , take  $y_N^{\pi, R_w}(\cdot) = f(\cdot)$ .

▷ Iteration : for  $k = N - 1, \dots, 0$ , solve the  $d$  least-squares problems

$$\alpha_{l,k}^M = \arg \inf_{\alpha} \frac{1}{M} \sum_{m=1}^M |y_{k+1}^{\pi, R_w, M}(X_{t_{k+1}}^{\pi, m}) \frac{[\Delta W_{l,k}^m]_w}{\Delta_k} - \alpha \cdot p_{l,k}(X_{t_k}^{\pi, m})|^2$$

and set  $z_{l,k}^{\pi, R_w, M}(\cdot) = [\alpha_{l,k}^M \cdot p_{l,k}(\cdot)]_z$ .

Then compute  $\alpha_{0,k}^M$  as the minimizer of

$$\sum_{m=1}^M |y_{k+1}^{\pi, R_w, M}(X_{t_{k+1}}^{\pi, m}) + \Delta_k g(t_k, X_{t_k}^{\pi, m}, y_{k+1}^{\pi, R_w, M}(X_{t_{k+1}}^{\pi, m}), z_k^{\pi, R_w, M}(X_{t_{k+1}}^{\pi, m})) - \alpha \cdot p_{0,k}(X_{t_k}^{\pi, m})|^2$$

and define  $y_k^{\pi, R_w, M}(\cdot) = [\alpha_{0,k}^M \cdot p_{0,k}(\cdot)]_y$ .

**Error analysis.** We now turn to the error estimates. The analysis combines the BSDE techniques (a priori estimates using stochastic calculus), regression tools as those exposed in Paragraph 5.3.2, but there is a slight difference which actually requires a significant improvement in the arguments. Since we use a single set of independent paths, the "responses"  $(y_{k+1}^{\pi, R_w, M}(X_{t_{k+1}}^{\pi, m})[\Delta W_{l,k}^m]_w)_{0 \leq m \leq M}$  are not independent, because of their dependence through the function  $y_{k+1}^{\pi, R_w, M}$ . To overcome this lack of independence in the proof, we shall replace the random function  $y_{k+1}^{\pi, R_w, M}$  by a deterministic neighbor: of course, there is a complexity to recover the different function spaces to provide close neighbors, and the covering numbers are well controlled using the Vapnik-Chervonenkis dimension, when the function spaces are bounded. This is the technical reason why we have truncated the Brownian increments. We now state a result regarding the global error, see [LGW06] for full details.

**Theorem 5.6** *Under the previous notations and assumptions, there is a constant  $C > 0$  (independent on  $R_w$  and  $N$ ) such that we have*

$$\begin{aligned}
& \max_{0 \leq k \leq N} \mathbb{E} |Y_{t_k}^{\pi, R_w} - y_k^{\pi, R_w, M}(X_{t_k}^\pi)|^2 + \Delta_k \sum_{k=0}^{N-1} \mathbb{E} |Z_{t_k}^{\pi, R_w} - z_k^{\pi, R_w, M}(X_{t_k}^\pi)|^2 \\
& \leq C \underbrace{\frac{C_\star^2 \log(M)}{M} \sum_{k=0}^{N-1} \sum_{l=0}^d K_{l,k}}_{\text{statistical error}} + CN^{-1} \\
& + C \underbrace{\sum_{k=0}^{N-1} \left\{ \inf_{\alpha} \mathbb{E} |y_k^{\pi, R_w}(X_{t_k}^\pi) - \alpha \cdot p_{0,k}(X_{t_k}^\pi)|^2 + \sum_{l=1}^d \inf_{\alpha} \mathbb{E} |\sqrt{\Delta_k} z_{l,k}^{\pi, R_w}(X_{t_k}^\pi) - \alpha \cdot p_{l,k}(X_{t_k}^\pi)|^2 \right\}}_{\text{approximation error of function class}} \\
& + CC_\star^2 N \sum_{k=0}^{N-1} \left\{ K_{0,k} \exp \left( - \frac{M}{C C_\star^2 K_{0,k} N^3} + CK_{0,k+1} \log(C C_\star (K_{0,k})^{\frac{1}{2}} N^{\frac{3}{2}}) \right) \right. \\
& \quad + N^{-1} K_{l,k} \exp \left( - \frac{M}{C C_\star^2 R_w^2 K_{l,k} N^2} + CK_{0,k+1} \log(C C_\star R_w (K_{l,k})^{\frac{1}{2}} N) \right) \\
& \quad \left. + \exp \left( CK_{0,k} \log(C C_\star N^{\frac{3}{2}}) - \frac{M}{C C_\star^2 N^3} \right) \right\}.
\end{aligned}$$

The last term between brackets is due to dependent regression problems. Those upper bounds are available under very mild assumptions on the model, therefore it can easily be applied to most of the usual applications.

**Parameter tuning.** We conclude this analysis by providing an example of how to choose appropriately the parameters  $N$ ,  $K_{l,k}$  and  $M$ . Our objective is to achieve a global error of order  $\varepsilon = \frac{1}{N}$  for  $\max_{0 \leq k \leq N} \mathbb{E} |Y_{t_k}^{\pi, R_w} - y_k^{\pi, R_w, M}(X_{t_k}^N)|^2 + \Delta_k \sum_{k=0}^{N-1} \mathbb{E} |Z_{t_k}^{\pi, R_w} - z_k^{\pi, R_w, M}(X_{t_k}^N)|^2$ .

For the vector spaces, we consider those generated by functions that are constant on disjoint hypercubes of small edge. Since  $X^\pi$  has exponential moments, it is easy to restrict the partitioning to a compact set of  $\mathbb{R}^d$  and analyze the induced error. If the edge of the hypercube is like  $N^{-1}$ , the vector spaces have dimension  $K_{l,k} \sim N^{-d}$  up to logarithmic terms. Due to Proposition 5.5, the terms from *approximation error of function class* are  $O(N^{-2})$  and they sum up to give a contribution  $O(N^{-1})$ . A quick inspection of the upper bounds shows that the highest constraint on  $M$  comes from the last term: we obtain  $M \sim cN^{3+2d}$  for  $c$  large enough, up to logarithmic terms. The complexity of the scheme is of order  $NM$  (still neglecting the log terms), because the computation of all regression coefficients at a give date has a computational cost  $O(M \log(N))$  due to our specific choice of function basis. Hence, the global complexity is

$$\mathcal{C} \sim \varepsilon^{-\frac{1}{4+2d}}$$

up to logarithmic terms.



In practice, the algorithm has been performed on a computer up to dimension  $d = 10$  with satisfactory results and rather short computational times (less than one minute). There are several possible improvements to this basic version of the algorithm.

- Using *local duplicating of paths* reduces the last term in Theorem 5.6 and thus, it improves the final complexity given the expected accuracy, see [GL06].
- We can use variance reduction techniques, see [BS12].
- Instead of writing the DPE between  $t_i$  and  $t_{i+1}$ , it can be written between  $t_i$  and  $T$ : it has the surprising effect (mathematically justified) to reduce the propagation of errors in the DPE. This scheme is called MDP scheme (for Multi step forward Dynamic Programming equation) and it is studied in [GT12].

**Complementary references:** for theoretical aspects, see [PP92], [EKP<sup>+</sup>97], [Par98], [MY99]; for applications, see [EHM08] and [EPQ97]; for numerics, see [BP03], [Zha04], [BT04], [GLW05], [LGW06], [BD07], [GL10], [CM10]. This list is not exhaustive.

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